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Laplace Transform Inversion and Time-Discretization Methods for Evolution Equations

Koray Ozer

Louisiana State University and Agricultural and Mechanical College

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LAPLACE TRANSFORM INVERSION AND
TIME-DISCRETIZATION METHODS FOR EVOLUTION EQUATIONS

A Dissertation

Submitted to the Graduate Faculty of the
Louisiana State University and
Agricultural and Mechanical College
in partial fulfillment of the
requirements for the degree of
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by
Koray Özer
B.S., Koç University, Istanbul, Turkey, 2000
M.S., Louisiana State University, USA, 2004
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Table of Contents

Acknowledgments	ii
Abstract	iv
Introduction	1
Chapter 1: Time-Discretization Methods for Operator Semigroups	5
1.1 An Overview of Semigroups	5
1.2 Rational Approximations of the Exponential Function	22
1.3 Rational Approximations of Operator Semigroups	38
Chapter 2: Numerical Inversion of the Laplace Transform	51
2.1 Rational Inversion of the Laplace Transform	51
2.2 Subdiagonal Padé Inversion of the Laplace Transform	57
2.3 Restricted Padé Inversion of the Laplace Transform	66
2.4 Applications to the Inhomogeneous Abstract Cauchy Problem	73
References	87
Vita	91

Abstract

In this dissertation, we introduce Post-Widder-type inversion methods for the Laplace transform based on \mathcal{A} -stable rational approximations of the exponential function of order $m \geq 1$. It is shown that a bounded, continuous function u can be approximated in terms of its Laplace transform \hat{u} by expressions

$$\sum_{\substack{0 \leq j \leq n-1 \\ 1 \leq k \leq m}} a_{j,k} \left(\frac{n}{t}\right)^{j+1} \hat{u}^{(j)}\left(b_k \frac{n}{t}\right),$$

where the coefficients $a_{j,k}, b_k$ are independent of u and $\operatorname{Re}(b_k) > 0$. If u is analytic, continuous, and bounded in a sectorial region containing the half-line $[0, \infty)$, then the mathematical approximation error is bounded by $C \frac{1}{n^m} \|u\|_\infty$ (with the constant C being independent of t and u); if u is $(m+1)$ -times continuously differentiable and bounded, then the error is bounded by $C t \frac{1}{n^m} \|u^{(m+1)}\|_\infty$; if u is continuously differentiable and bounded, then the error is bounded by $C t \frac{1}{n^\beta} \|u'\|_\infty$ for some $\frac{1}{2} \leq \beta < 1$. In particular, if u is sufficiently smooth, then n , the order of the derivatives of \hat{u} , can be kept low by taking rational approximations of the exponential function of high approximation order m . Since the results hold for Banach-space-valued functions, they yield efficient time-discretization methods for evolution equations of convolution type; e.g., linear first and higher order abstract Cauchy problems, inhomogeneous Cauchy problems, delay equations, Volterra and integro-differential equations, and problems that can be re-written as an abstract Cauchy problem $u'(t) = Au(t), u(0) = x, t \in [0, T]$ on an appropriate state space X .

Introduction

The starting point for this dissertation project are the results due to Hersh and Kato [26], Brenner and Thomée [7], Larsson, Thomée and Wahlbin [40], Hansbo [25], and Crouzeix, Larsson, Piskarev and Thomée [11] concerning time discretization methods for evolution equations that can be given the abstract formulation as a homogeneous abstract Cauchy problem

$$\dot{u}(t) = Au(t), \quad u(0) = x, \quad t \geq 0, \quad (1)$$

where A is the generator of a strongly continuous semigroup $\{T(t)\}_{t \geq 0}$ on a Banach space X . Abstract Cauchy problems arise, for example, from initial and boundary value problems for partial differential equations, Volterra integral equations, and delay equations. The aim of this dissertation is to generalize their results and methods to more general classes of evolution equations, in particular, to inhomogeneous problems

$$\dot{u}(t) = Au(t) + f(t), \quad u(0) = x, \quad t \geq 0, \quad (2)$$

where $f : [0, \infty) \rightarrow X$ is a sufficiently smooth forcing term.

The original dissertation research plan started out with the ‘semigroup approach’ to the inhomogeneous problem by rewriting (2) as a homogeneous Cauchy problems (1) on a properly chosen state space \mathcal{X} . More precisely, assuming that $f \in C_0(\mathbb{R}^+, X)$, we first write (2) as

$$w'(t) = \mathfrak{A}w(t), \quad w(0) = (x, f),$$

where

$$\mathfrak{A} = \begin{pmatrix} A & \delta_0 \\ 0 & d/ds \end{pmatrix}$$

on a new state space $\mathcal{X} := X \times C_0(\mathbb{R}^+, X)$. Here, $(A, D(A))$ is the generator of a strongly continuous semigroup $\{T(t)\}_{t \geq 0}$ on Banach space X and δ_0 is the point evaluation in 0. Then, we show that the new operator $(\mathfrak{A}, D(\mathfrak{A}))$ with

$$D(\mathfrak{A}) := D(A) \times C_0^1(\mathbb{R}^+, X)$$

generates a strongly continuous semigroup $\{\mathfrak{T}(t)\}_{t \geq 0}$ on \mathcal{X} defined by

$$\mathfrak{T}(t) := \begin{pmatrix} T(t) & R(t) \\ 0 & S(t) \end{pmatrix},$$

where $\{S(t)\}_{t \geq 0}$ is the (left) shift semigroup on $C_0(\mathbb{R}^+, X)$ and $R(t) : C_0(\mathbb{R}^+, X) \rightarrow X$ is defined as

$$R(t)f := \int_0^t T(t-s)f(s) ds \quad \text{for } f \in C_0(\mathbb{R}^+, X).$$

While pursuing this approach, it soon became apparent that a ‘Laplace transform’ approach to (2) might be more appropriate. It is one of the main results of my dissertation that an adequate tool to study time-discretization procedures for convolution-type evolution equations is a set of entirely new, numerically and analytically effective and efficient inversion formulas for the Laplace transform.

By applying the results of [7], [11], [25], [26], [40] (see Sections 1.2 and 1.3) to the Cauchy problem

$$w_t(t, s) = w_s(t, s), \quad w(0, s) = u(s), \quad s, t \geq 0,$$

for $u \in \mathcal{C}_0(\mathbb{R}^+, X)$, $\mathcal{C}_b(\mathbb{R}^+, X)$, or $C_b(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X)$ ¹ and the associated shift semigroup $T(t)u(s) := u(t + s)$, we introduce Post-Widder-type inversion methods for the Banach-space-valued Laplace transform based on \mathcal{A} -stable rational approximations of the exponential function of approximation order $m \geq 1$; i.e., $r = \frac{P}{Q}$ for some polynomials P, Q with $\deg(P) \leq \deg(Q)$, $|r(z) - e^z| \leq C|z|^{m+1}$ for $|z|$ sufficiently small, and $|r(z)| \leq 1$ for $\operatorname{Re}(z) \leq 0$.

By using the fact that the generator $D = \frac{d}{ds}$ of the (left) shift semigroup $T(t)u : s \rightarrow u(t + s)$ satisfies

$$R(\lambda, D)u(s) = (\lambda I - D)^{-1}u(s) = \int_0^\infty e^{-\lambda t} u(t + s) ds,$$

and thus

$$\begin{aligned} T(t)u(0) &= u(t), \\ R(\lambda, D)u(0) &= \hat{u}(\lambda), \end{aligned}$$

where $\hat{u}(\lambda)$ denotes the Laplace transform of u , the aforementioned time-discretization methods imply that the inverse Laplace transform u of a given analytic function \hat{u} can be approximated by expressions of the form

$$\sum_{\substack{0 \leq j \leq n-1 \\ 1 \leq k \leq s_m}} a_{j,k} \left(\frac{n}{t}\right)^{j+1} \hat{u}(j)(b_k \frac{n}{t}), \quad (3)$$

where the coefficients $a_{j,k}, b_k$ are predetermined by the rational approximation scheme r and independent of u . In the literature, the inversion of the Laplace transform is often considered to be

¹ $\mathcal{C}_b(\mathbb{R}^+, X)$ denotes the Banach space of bounded and continuous functions from \mathbb{R}^+ into X , $\mathcal{C}_0(\mathbb{R}^+, X) := \{u \in \mathcal{C}_b(\mathbb{R}^+, X) : u(\infty) = 0\}$, $\Sigma_\theta := \{z \in \mathbb{C} \setminus \{0\} : |\arg(z)| < \theta\}$, $H(\Sigma_\theta, X) := \{u : \Sigma_\theta \rightarrow X \text{ analytic}\}$, and $C_b(\overline{\Sigma_\theta}, X)$ the space of all bounded, continuous functions from $\overline{\Sigma_\theta}$ into X .

a fundamentally ill-posed problem. We show that this is not the case; i.e., the Laplace transform inversions (3) come with sharp error estimates for the mathematical approximation error

$$E(n, u, t) := \left\| \sum_{\substack{0 \leq j \leq n-1 \\ 1 \leq k \leq s_m}} a_{j,k} \left(\frac{n}{t}\right)^{j+1} \hat{u}(j)(b_k \frac{n}{t}) - u(t) \right\|. \quad (4)$$

If u is an analytic and bounded function in $C_b(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X)$, then there is a constant C (independent of n, u, t) such that

$$E(n, u, t) \leq C \frac{1}{n^m} \|u\|_\infty. \quad (5)$$

If $u, u^{(m+1)} \in \mathcal{C}_b(\mathbb{R}^+, X)$, then

$$E(n, u, t) \leq C t \left(\frac{t}{n}\right)^m \|u^{(m+1)}\|_\infty, \quad (6)$$

where the actual numerical error in concrete examples is considerably less. In particular, if u is smooth, then n , the order of the derivatives of \hat{u} , can be kept low by taking rational approximations r of the exponential function of high approximation order m . Since the results hold for Banach space valued functions, they are applicable to approximate solutions u of evolution equations of convolution type (e.g. linear first and higher order abstract Cauchy problems, inhomogeneous Cauchy problems, delay equations, Volterra and integro-differential equations, etc.) as well as to all problems (linear and nonlinear) that can be re-written as a linear, well- or ill-posed abstract Cauchy problem $\dot{u}(t) = Au(t)$, $u(0) = x$, $t \in [0, \tau]$ on an appropriate state space \mathcal{X} .

Chapter 1

Time-Discretization Methods for Operator Semigroups

In Section 1.1, we give a brief introduction to the theory of operator semigroups. After presenting the basics of strongly continuous semigroups such as their generators, resolvents, the Hille-Yosida generation theorem and the Hille-Phillips functional calculus, we give some attention to analytic semigroups and bi-continuous semigroups. In particular, we introduce and discuss the basic properties of bi-continuous analytic semigroups which will be needed later on. In Section 1.2, rational approximation schemes of the exponential function, such as Padé and restricted Padé approximants will be illustrated with examples. Moreover, we introduce and discuss rational best-approximations of the exponential function. In Section 1.3, we collect the main results on rational approximations of strongly continuous semigroups due to Brenner and Thomée [7] based on work of Hersh and Kato [26]. We extend the uniform error estimates for analytic semigroups due to Larsson, Thomée and Wahlbin [40] and Crouzeix, Larsson, Piskarev and Thomée [11] to bi-continuous analytic semigroups - a fact that will be of critical importance in Chapter 2 where we present new inversion methods for Laplace transforms of bounded analytic functions. To have the findings at hand when discussing the corresponding Laplace transform inversion results, we recall in Section 1.3 extensions of the Brenner-Thomée results due to Kovács [35], stability results obtained by Hansbo [25], and stabilization methods due to McAllister and Neubrander [42]. Finally, we shall establish rational best-approximation results through the Hille-Phillips functional calculus.

1.1 An Overview of Semigroups

For a detailed treatment of strongly continuous semigroups and analytic semigroups, see, for example, [17], [41]; for bi-continuous semigroups, see [19], [37].

Let X denote a Banach space and let $\mathcal{L}(X)$ denote the collection of bounded operators on X . We say that $\{T(t)\}_{t \geq 0}$ is a semigroup of bounded linear operators on X if the operators $T(t)$ are in $\mathcal{L}(X)$ for all $t \in \mathbb{R}^+$ and satisfy the semigroup property

$$(i) \quad T(0) = I,$$

$$(ii) \quad T(t)T(s) = T(t+s), \quad s, t \geq 0.$$

A semigroup $\{T(t)\}_{t \geq 0}$ of bounded linear operators on X is a strongly continuous semigroup if

$$(iii) \quad \lim_{t \downarrow 0} T(t)x = x \quad \text{for every } x \in X.$$

It can be easily seen that the properties (i)-(iii) imply that the orbit maps $t \mapsto T(t)x$ are continuous on $[0, \infty)$ for all $x \in X$.

The linear operator A defined on the domain

$$D(A) = \left\{ x \in X : \lim_{t \downarrow 0} \frac{T(t)x - x}{t} \text{ exists} \right\}$$

by

$$Ax = \lim_{t \downarrow 0} \frac{T(t)x - x}{t} = \left. \frac{d^+ T(t)x}{dt} \right|_{t=0}$$

is the (*infinitesimal*) *generator* of the semigroup $\{T(t)\}_{t \geq 0}$.

As an immediate consequence of the semigroup properties and strong continuity, one obtains the following essential relation between a strongly continuous semigroup and its generator.

(i) If $x \in D(A)$, then $T(t)x \in D(A)$ and

$$\frac{d}{dt} T(t)x = T(t)Ax = AT(t)x \quad \text{for all } t \geq 0. \quad (1.1)$$

In particular, for all $t \geq 0$ and $x \in D(A)$,

$$T(t)x - x = \int_0^t T(s)Ax \, ds.$$

(ii) For every $t \geq 0$ and $x \in X$, one has

$$\int_0^t T(s)x \, ds \in D(A)$$

and

$$T(t)x - x = A \int_0^t T(s)x \, ds. \quad (1.2)$$

With the help of the statements above, it can be easily deduced that the generator $(A, D(A))$ of a strongly continuous semigroup $\{T(t)\}_{t \geq 0}$ on a Banach space X is closed and densely defined, see, for example, Corollary I.2.5 in [46]. Moreover, if $\{S(t)\}_{t \geq 0}$ is another strongly continuous semigroup with the same generator $(A, D(A))$, then $S(t) = T(t)$ for all $t \geq 0$.

As a first example of a strongly continuous semigroup, let $A \in \mathbb{C}^{n \times n}$ and consider

$$T(t) := e^{tA} := \sum_{n=0}^{\infty} \frac{t^n}{n!} A^n = \lim_{n \rightarrow \infty} \left(I + \frac{t}{n} A\right)^n = \lim_{n \rightarrow \infty} \left(I - \frac{t}{n} A\right)^{-n}$$

Then the map $t \rightarrow T(t)$ is an entire function from \mathbb{C} into $\mathcal{L}(X)$ with (bounded) generator A and $D(A) = X = \mathbb{C}^n$. The most fundamental semigroup with an unbounded generator A is given by the (left) shift semigroup

$$(T(t)f)(s) := f(s+t), \quad s \in \mathbb{R}.$$

This semigroup will play an essential role later on in obtaining the novel method for the inversion of the Laplace transform. Having applications to Laplace transform theory in mind, we consider the shift semigroup on a sup-norm space \mathcal{X} , where \mathcal{X} is either

- $C_{ub}(\mathbb{R}^+, X)$, the Banach space of bounded, uniformly continuous functions from \mathbb{R}^+ into a Banach space X ,
- $C_0(\mathbb{R}^+, X)$, the Banach space of continuous functions from \mathbb{R}^+ into X vanishing at infinity,
- $C_b(\mathbb{R}^+, X)$, the Banach space of bounded, continuous functions from \mathbb{R}^+ into X .

It is easy to see that the shift semigroup is strongly continuous on $\mathcal{X} = C_{ub}(\mathbb{R}^+, X)$ and $\mathcal{X} = C_0(\mathbb{R}^+, X)$. The generator of the shift semigroup is $Af = f'$ with maximal domain

$$D(A) = \{f \in \mathcal{X} : f \text{ is continuously differentiable and } f' \in \mathcal{X}\}.$$

However, if $\mathcal{X} = C_b(\mathbb{R}^+, X)$, then the shift semigroup is no longer strongly continuous. To see this, let $0 \neq x_0 \in X$ with $\|x_0\| = 1$ and define $f(t) := \sin(t^2)x_0$. Then

$$\|T(t_1)f - T(t_2)f\| = \sup_{s \geq 0} |\sin(t_1 + s)^2 - \sin(t_2 + s)^2| = 2 \quad \text{if } t_1 \neq t_2.$$

Thus, $t \mapsto T(t)f$ is nowhere continuous (in fact, it is not even measurable since it is not almost separably valued, see Theorem 1.1.1 in [2]). However, if one endows $C_b(\mathbb{R}^+, X)$ with the topology of uniform convergence on compact sub-intervals of $[0, \infty)$, then $t \mapsto T(t)f$ is continuous for all $f \in C_b(\mathbb{R}^+, X)$. It is this observation that leads to the definition of bi-continuous semigroups below. The shift semigroup plays an important role in Laplace transform theory since the fundamental equality

$$f(t) = T(t)f(0) = \langle \mu_0, T(t)f \rangle$$

(where $\langle \mu_0, g \rangle := g(0)$) allows to translate the study of functions $f \in C_b(\mathbb{R}^+, X)$ (or $C_{ub}(\mathbb{R}^+, X)$, $C_0(\mathbb{R}^+, X)$) into the study of the linear shift operators $T(t)$ (evaluated at f at $s = 0$). In particular, every approximation result for strongly continuous semigroups will translate into an approximation result for continuous functions $f \in C_b(\mathbb{R}^+, X)$ (or $C_{ub}(\mathbb{R}^+, X)$, $C_0(\mathbb{R}^+, X)$) if applied to the (left) shift semigroup on either of these spaces.

So far we have seen that every strongly continuous semigroup has a generator which determines the semigroup uniquely. For applications of semigroup theory to evolution equations, one needs to know how to determine whether a given operator A on a Banach space X is *suitable* to be the generator of some strongly continuous semigroup $\{T(t)\}_{t \geq 0}$. Before giving the characterization theorem, we need the following essential result.

Let $\{T(t)\}_{t \geq 0}$ be a strongly continuous semigroup on the Banach space X . Then there exists constants $M > 0$ and $\omega \geq 0$ such that

$$\|T(t)\| \leq Me^{\omega t} \quad \text{for all } t \geq 0. \quad (1.3)$$

To see this observe that the continuity of $t \mapsto T(t)x$ implies local boundedness of $t \mapsto T(t)x$ and thus, by the *principle of uniform boundedness*, the local boundedness of $t \mapsto \|T(t)\|$. Choose $M \geq 1$ such that $\|T(s)\| \leq M$ for $s \in [0, 1]$. Let $t = s + n$ for $s \in [0, 1)$ and $n \in \mathbb{N}$. Then

$$\begin{aligned} \|T(t)\| &= \|T(s + n)\| \leq \|T(s)\| \|T(1)\|^n \\ &\leq M^{n+1} = Me^{n \ln M} \leq Me^{\omega t} \quad \text{with } \omega := \ln M. \end{aligned}$$

Since the generator $(A, D(A))$ of a strongly continuous operator is always a closed operator, by the Closed Graph Theorem, if $(A, D(A))$ is bijective, its inverse becomes a bounded operator on X . As we will see next, the semigroup properties together with (1.3) imply that the resolvent of the generator A of a strongly continuous semigroup is given by the Laplace transform of $t \mapsto T(t)x$.

Let $(A, D(A))$ be a closed operator on a Banach space X . The resolvent set of A is defined by

$$\rho(A) := \{\lambda \in \mathbb{C} : \lambda - A \text{ is bijective}\},$$

and

$$\sigma(A) := \mathbb{C} - \rho(A)$$

denotes the spectrum of A . For $\lambda \in \rho(A)$, we call $R(\lambda, A) := (\lambda - A)^{-1}$ the resolvent of A at λ .

If $\{T(t)\}_{t \geq 0}$ is a strongly continuous semigroup satisfying (1.3), then the resolvent of the generator is given by the Laplace transform of the semigroup for $\operatorname{Re}(\lambda) > \omega$. That is, if $(A, D(A))$ is the generator of a strongly continuous semigroup $\{T(t)\}_{t \geq 0}$ on a Banach space X , then for every $\lambda \in \mathbb{C}$ with

$$\operatorname{Re}(\lambda) > \omega_0(A) := \inf\{\omega \in \mathbb{R} : \exists M > 0 \text{ such that } \|T(t)\| \leq Me^{\omega t} \forall t \geq 0\}$$

we have $\lambda \in \rho(A)$ and

$$R(\lambda, A)x = \int_0^\infty e^{-\lambda s} T(s)x \, ds \quad \text{for all } x \in X. \quad (1.4)$$

The abscissa $\omega_0(A) = \lim_{t \rightarrow 0} \frac{1}{t} \ln \|T(t)\|$ is said to be the *growth bound* of the semigroup $\{T(t)\}_{t \geq 0}$.

Moreover, since all resolvents satisfy

$$R(\lambda, A)^{n+1} = (-1)^n \frac{1}{n!} R(\lambda, A)^{(n)}, \quad (1.5)$$

it follows from (1.4) that

$$R(\lambda, A)^{n+1}x = (-1)^n \frac{1}{n!} \frac{d^n}{d\lambda^n} \int_0^\infty e^{-\lambda t} T(t)x dt \quad (1.6)$$

$$= \int_0^\infty e^{-\lambda t} \frac{t^n}{n!} T(t)x dt \quad (1.7)$$

for all $x \in X$ and $\operatorname{Re}(\lambda) > \omega$. In particular, if $\|T(t)\| \leq M e^{\omega t}$, then

$$\|R(\lambda, A)^{n+1}x\| \leq M \int_0^\infty e^{-(\operatorname{Re}(\lambda) - \omega)t} \frac{t^n}{n!} \|x\| dt = \frac{M}{(\operatorname{Re}(\lambda) - \omega)^{n+1}} \|x\|.$$

This leads to the fundamental characterization theorem in semigroup theory which provides necessary and sufficient conditions for A to be the generator of a strongly continuous semigroup.

Theorem 1.1 (Hille-Yosida). *Let $(A, D(A))$ be a linear operator on a Banach space X and let $\omega \in \mathbb{R}$, $M \geq 1$ be constants. Then the following properties are equivalent.*

(i) $(A, D(A))$ generates a strongly continuous semigroup $T(t)$ satisfying

$$\|T(t)\| \leq M e^{\omega t} \quad \text{for all } t \geq 0.$$

(ii) $(A, D(A))$ is closed, densely defined, and for every $\lambda > \omega$ one has $\lambda \in \rho(A)$ and

$$\|R(\lambda, A)^n\| \leq \frac{M}{(\lambda - \omega)^n} \quad \text{for all } n \in \mathbb{N}.$$

(iii) $(A, D(A))$ is closed, densely defined, and for every $\lambda \in \mathbb{C}$ with $\operatorname{Re}(\lambda) > \omega$ one has $\lambda \in \rho(A)$ and

$$\|R(\lambda, A)^n\| \leq \frac{M}{(\operatorname{Re}(\lambda) - \omega)^n} \quad \text{for all } n \in \mathbb{N}.$$

The basic notions of strongly continuous semigroups we have described so far, in point of fact, form the focal role in solving initial value problems.

Let X be a Banach space, let $A : D(A) \subseteq X \rightarrow X$ a closed linear operator, and let $x \in X$. The initial value problem

$$(ACP) \begin{cases} \dot{u}(t) = Au(t) & \text{for } t \geq 0, \\ u(0) = x \end{cases}$$

is called the abstract Cauchy problem associated to $(A, D(A))$ with the initial value $x \in X$.

A function $u : \mathbb{R}^+ \rightarrow X$ is called a classical solution of (ACP) if u is continuously differentiable, $u(t) \in D(A)$ for all $t \geq 0$, and (ACP) holds. A continuous function $u : \mathbb{R}^+ \rightarrow X$ is called a mild solution of (ACP) if $\int_0^t u(s)ds \in D(A)$ and

$$u(t) = x + A \int_0^t u(s)ds \quad \text{for all } t \geq 0.$$

Since A is assumed to be closed, every classical solution is a mild solution. Moreover, it follows easily from (1.1) and (1.2) that if $(A, D(A))$ generates a strongly continuous semigroup $\{T(t)\}_{t \geq 0}$, then, for every $x \in D(A)$, the function

$$u : t \mapsto u(t) := T(t)x$$

is the unique classical solution of (ACP) with initial value x . In fact, for a closed operator $A : D(A) \subseteq X \rightarrow X$, the associated abstract Cauchy problem is well-posed if and only if $(A, D(A))$ generates a strongly continuous semigroup on X . That is, if A is a closed operator on a Banach space X , then the following statements are equivalent.

- (i) For all $x \in X$ there exists a unique mild solution of (ACP).
- (ii) The operator A generates a strongly continuous semigroup.

(iii) $\rho(A)$ is non-empty and for all $x \in D(A)$ there exists a unique classical solution of (ACP).

When these assertions hold, for all $x \in X$ the mild solution of the abstract Cauchy problem is given by $u(t) = T(t)x$. Therefore, to solve an (ACP) means to show that the operator $(A, D(A))$ generates a strongly continuous semigroup. Before turning our attention to analytic semigroups, let us consider again the shift semigroup $T(t)f(s) := f(t+s)$ on one of the spaces $\mathcal{X} := C_{ub}(\mathbb{R}^+, X)$ (or $C_b(\mathbb{R}^+, X)$, $C_0(\mathbb{R}^+, X)$). Then the generator of the contraction semigroup $\{T(t)\}_{t \geq 0}$ is given by $Af = f'$ with maximal domain $D(A) = \{f \in \mathcal{X} : f \text{ is continuously differentiable and } f' \in \mathcal{X}\}$ and with resolvent

$$R(\lambda, A)f(s) = \int_0^\infty e^{-\lambda t} T(t)f(s) dt = \int_0^\infty e^{-\lambda t} f(t+s) dt,$$

where $f \in \mathcal{X}$, $s \geq 0$, and $\operatorname{Re}(\lambda) > 0$. In particular, the Laplace transform

$$\hat{f}(\lambda) := \int_0^\infty e^{-\lambda t} f(t) dt$$

of $f \in \mathcal{X}$ is given by

$$R(\lambda, A)f(0) = \int_0^\infty e^{-\lambda t} T(t)f(0) dt = \int_0^\infty e^{-\lambda t} f(t) dt = \hat{f}(\lambda).$$

Thus, since the shift semigroup satisfies

$$\begin{aligned} f(t) = T(t)f(0) &= \langle \mu_0, T(t)f \rangle \\ \hat{f}(\lambda) = R(\lambda, A)f(0) &= \langle \mu_0, R(\lambda, A)f \rangle \end{aligned} \tag{1.8}$$

with $\langle \mu_0, g \rangle := g(0)$ for $g \in \mathcal{X}$, we see that every approximation result for strongly continuous semigroups $\{T(t)\}_{t \geq 0}$ in terms of the resolvents $\{R(\lambda, A)\}_{\operatorname{Re} \lambda > \omega}$ of the generator $(A, D(A))$ yields, if applied to the shift semigroup on the sup-norm spaces \mathcal{X} , an approximation result of

$t \mapsto f(t)$ in terms of its Laplace transform $\lambda \mapsto \hat{f}(\lambda)$. We will further explore this powerful idea in Chapter 2.

Now, we introduce another class of semigroups, namely, analytic semigroups. So far we have dealt with semigroups whose domain is the non-negative real axis. We shall now consider the possibility of extending the domain to sectorial regions in the complex plane that include the non-negative real axis. This class of semigroups plays an important role in the theory of evolution equations, indeed; the treatment of linear and non-linear parabolic partial differential equations is based to a large degree on the theory of analytic semigroups.

Let $\Sigma_\theta := \{z \in \mathbb{C} - \{0\} : |\arg(z)| < \theta\}$ be the sector in the complex plane of angle $\theta \in (0, \pi]$.

A family of bounded linear operators $\{T(z)\}_{z \in \Sigma_\theta \cup \{0\}}$ on a Banach space X is called an analytic semigroup of angle θ if

- (i) $T(0) = I$ and $T(z_1 + z_2) = T(z_1)T(z_2)$ for all $z_1, z_2 \in \Sigma_\theta$,
- (ii) the map $z \mapsto T(z)$ is analytic on Σ_θ , and
- (iii) $\lim_{z \rightarrow 0, z \in \Sigma_{\theta'}} T(z)x = x$ for all $x \in X$ and $0 < \theta' < \theta$.

If, in addition,

- (iv) $\sup_{z \in \Sigma_{\theta'}} \|T(z)\| < \infty$ for every $0 < \theta' < \theta$,

then we call $\{T(z)\}_{z \in \Sigma_\theta \cup \{0\}}$ a bounded analytic semigroup.

Similar to the Hille-Yosida characterization theorem for generators of strongly continuous semigroups, we have the same issue of determining which properties of the generator A will guarantee that a given semigroup is an analytic semigroup. A closed linear operator A is said to be a θ -sectorial operator on Banach space X if there exists $0 < \theta \leq \pi/2$ such that the sector $\Sigma_{\pi/2+\theta}$ is contained in the resolvent set $\rho(A)$, and if for each $\epsilon \in (0, \theta)$ there exists M_ϵ such that

$$\|R(\lambda, A)\| \leq \frac{M_\epsilon}{|\lambda|} \quad \text{for all } 0 \neq \lambda \in \bar{\Sigma}_{\pi/2+\theta-\epsilon}.$$

It is one of the key results of analytic semigroup theory that for an operator $(A, D(A))$ on Banach space X the following assertions are equivalent (see, e.g. Corollary 3.7.12 in [2])

- (i) A generates a bounded analytic semigroup $\{T(z)\}_{z \in \Sigma_\theta \cup \{0\}}$.
- (ii) The operators $e^{\pm i\delta} A$ generate bounded, strongly continuous semigroups on X for all $0 < \delta < \theta$
- (iii) A is densely defined and θ -sectorial.

Moreover, A generates a bounded analytic semigroup $\{T(z)\}_{z \in \Sigma_\theta \cup \{0\}}$ for some $0 < \theta \leq \pi/2$ if and only if A generates a bounded strongly continuous semigroup $\{T(t)\}_{t \geq 0}$ on X and there exists a constant $C \geq 0$ such that

$$\|R(r + is, A)\| \leq \frac{C}{|s|}$$

for all $r > 0$ and $0 \neq s \in \mathbb{R}$.

Because of the aforementioned importance of the semigroup on sup-norm spaces in applications to Laplace transform theory, we illustrate analytic semigroups by giving an example of a sup-norm space on which the shift $t \mapsto T(t)f = f(t + \cdot)$ is analytic. Let $C_{ub}(\bar{\Sigma}_\theta, X)$ denote the space of all bounded, uniformly continuous functions on a closed sector $\bar{\Sigma}_\theta$, $0 < \theta \leq \pi/2$ with values in a Banach space X and let $H(\Sigma_\theta, X)$ be the space of all X -valued analytic functions in Σ_θ . Then

$$F_{ub}^\infty(\Sigma_\theta, X) := C_{ub}(\bar{\Sigma}_\theta, X) \cap H(\Sigma_\theta, X) \tag{1.9}$$

equipped with sup-norm is a Banach space. The (left) shift semigroup $T(z)$ on $F_{ub}^\infty(\Sigma_\theta, X)$ is defined by

$$T(z)f(\omega) := f(z + \omega) \quad \text{for } \omega \in \bar{\Sigma}_\theta, z \in \Sigma_\theta \cup \{0\}.$$

As $F_{ub}^\infty(\Sigma_\theta, X)$ is a closed, invariant subspace of $C_{ub}(\bar{\Sigma}_\theta, X)$, it follows that $\{T(t)\}_{t \geq 0}$ is a strongly continuous semigroup and, as expected, the operator $A = d/dx$ is its generator with domain

$$D(A) := \{f \in F_{ub}^\infty(\Sigma_\theta, X) : Af \in F_{ub}^\infty(\Sigma_\theta, X)\}.$$

Since, $T_\alpha(t) := T(e^{i\alpha t})$ is a strongly continuous semigroup generated by $e^{i\alpha}A$ for each $|\alpha| < \theta$, it follows that $T(\cdot)$ is analytic semigroup on Σ_θ . For details, see [4].

We have already noted that the theory of strongly continuous semigroups was constructed so as to treat initial value problems for partial differential equations. On the other hand, there are many situations in which the corresponding semigroup is not strongly continuous; for examples, see [19], [37]. The need for a generalization of strongly continuous semigroups to deal with such problems has resulted in the development of *bi-continuous* semigroups.

The concept of bi-continuous semigroups was introduced by F. Kühnemund in her dissertation from 2001 (see [37]) and further developed by B. Farkas [19] and other authors since. Bi-continuous semigroups are a special case of the more general class of *semigroups in locally convex spaces* developed by H. Komatsu in 1964 (see [32]). We will refer heavily to Komatsu's original work when introducing the class of bi-continuous analytic semigroups at the end of this section.

As explained above (see (1.8)), for the purposes of this dissertation, for us the main examples of bi-continuous semigroups are the (left) shift semigroups $T(t)f(s) := f(t + s)$ on $\mathcal{X} = C_b(\mathbb{R}, X)$ or on $\mathcal{X} = F_b^\infty(\Sigma_\theta, X) := C_b(\bar{\Sigma}_\theta, X) \cap H(\Sigma_\theta, X)$. As shown above, in these spaces the orbits $t \mapsto T(t)f$, $t \geq 0$, are not continuous with respect to the sup-norm topology of \mathcal{X} , but only with respect to the coarser topology of uniform convergence on compact subsets of \mathbb{R}^+ , or $\bar{\Sigma}_\theta$.

In general, instead of requiring the continuity of the maps $t \mapsto T(t)x$ with respect to the norm topology of a Banach space X , the underlying main idea of the class of bi-continuous semigroups $\{T(t)\}_{t \geq 0}$, is to require the continuity of $t \mapsto T(t)x$ only in a locally convex Hausdorff topology that is coarser than the norm topology, but still fine enough to be norming for X .

More precisely, let X denote a Banach space which is equipped with a locally convex Hausdorff topology τ which is coarser than the norm topology. Such a topology is called *coherent* if the locally convex space (X, τ) is sequentially complete on norm-bounded sets (i.e., every $\|\cdot\|$ -bounded, τ -Cauchy sequence converges in X) and if the dual space $(X, \tau)'$ is norming for $(X, \|\cdot\|)$, that is,

$$\|x\| = \sup_{\substack{\psi \in (X, \tau)' \\ \|\psi\| \leq 1}} |\psi(x)|.$$

Let \mathcal{P} denote the family of seminorms that determines the locally convex Hausdorff topology τ . For simplicity, we shall assume that all seminorms $p \in \mathcal{P}$ satisfy $p(x) \leq \|x\|$ for all $x \in X$.

For example, let $\mathcal{X} = C_b(\mathbb{R}^+, X)$ and let τ be the topology of uniform convergence on compact subsets of \mathbb{R}^+ . Then τ is a locally convex Hausdorff topology determined by the seminorms $\{p_N\}_{N \in \mathbb{N}}$, where

$$p_N(f) := \sup_{s \in [0, N]} \|f(s)\| \leq \|f\|_\infty \quad \text{for all } f \in \mathcal{X}.$$

Clearly, if $f_n \rightarrow f$ uniformly on compact subsets of $[0, \infty)$ and $\|f_n\| \leq M$ for all $n \in \mathbb{N}$, then $f \in \mathcal{X}$. That is, (\mathcal{X}, τ) is sequentially complete on norm bounded subsets of \mathcal{X} . Moreover, since the point evaluations $\mu_a(f) := f(a)$ are continuous linear functionals on (\mathcal{X}, τ) with $\|\mu_a\| = 1$ and since $(\mathcal{X}, \tau)' \subseteq (\mathcal{X}, \|\cdot\|_\infty)'$, it follows that

$$\begin{aligned}
\|f\| &= \sup_{a \geq 0} \|f(a)\| = \sup_{a \geq 0} \|\mu_a(f)\| \\
&\leq \sup_{\substack{\psi \in (\mathcal{X}, \sigma)' \\ \|\psi\|=1}} \|\psi(f)\| \leq \sup_{\substack{\psi \in (\mathcal{X}, \|\cdot\|_\infty)' \\ \|\psi\|=1}} \|\psi(f)\| = f.
\end{aligned}$$

Thus, the dual space $(\mathcal{X}, \tau)'$ is norming for $(\mathcal{X}, \|\cdot\|_\infty)$ and τ is a coherent topology. It can easily be seen that these arguments extend immediately to the topology of uniform convergence on

$$\mathcal{X} = F_b^\infty(\Sigma_\theta, X) := C_b(\bar{\Sigma}_\theta, X) \cap H(\Sigma_\theta, X).$$

A semigroup $\{T(t)\}_{t \geq 0}$ of bounded linear operators on a Banach space X is called a bi-continuous semigroup (with respect to a coherent topology τ defined via a family \mathcal{P}_τ of seminorms) if

- (i) it is τ -strongly continuous, i.e., the map $t \mapsto T(t)x \in X$ is τ -continuous for each $x \in X$,
- (ii) $\{T(t)\}_{t \geq 0}$ is exponentially bounded; i.e., there exists $M \geq 1$ and $\omega \in \mathbb{R}$ such that $\|T(t)\| \leq Me^{\omega t}$ for all $t \geq 0$,
- (iii) $\{T(t)\}_{t \geq 0}$ is locally bi-equicontinuous, i.e., for every $t_0 \geq 0$, $\epsilon > 0$, $p \in \mathcal{P}_\tau$, and for every $\|\cdot\|$ -bounded sequence $\{x_n\}_{n \in \mathbb{N}}$ with $\tau - \lim x_n = x$, there exists $n_0 \in \mathbb{N}$ such that

$$\sup_{0 \leq t \leq t_0} p[T(t)(x_n - x)] \leq \epsilon \quad \text{for all } n \geq n_0.$$

As will be seen below, for the generator A of a bi-continuous semigroup $\{T(t)\}_{t \geq 0}$ the resolvent $R(\lambda, A)$ is given by the Laplace transform of the semigroup $\{T(t)\}_{t \geq 0}$ in the coarser topology. Therefore, all the principal Laplace transform based results obtained for strongly continuous semigroups (e.g., Hille-Yosida Theorem, Trotter-Kato Theorem, Chernoff Product Formula, Hille-Phillips Functional Calculus, etc.) can be attained for bi-continuous semigroups without too much difficulty. Before collecting these results, let us examine, once again, the shift semigroup.

Let X be a Banach space, $\mathcal{X} := C_b(\mathbb{R}^+, X)$ and let τ denote the coherent topology of uniform convergence on compact subsets of \mathbb{R}^+ . Then the shift semigroup $\{T(t)\}_{t \geq 0}$ is τ -continuous (this follows immediately from the fact that a continuous function is uniformly continuous on compact subsets). Since $\|T(t)\| \leq 1$, the shift semigroup is bi-continuous on \mathcal{X} (with respect to τ) if it is locally bi-equicontinuous. To see the bi-equicontinuity, let $\{f_n\}_{n \geq 1} \in \mathcal{X}$ with $\|f_n\| \leq M$ such that $f := \tau - \lim f_n$ exists. Let $p_N \in \mathcal{P}_\tau$ be given by $p_N(f) := \sup_{s \in [0, N]} \|f(s)\|$, let $0 \leq t \leq t_0 \leq M$ and $\epsilon > 0$ be given. Then, there exists $n_0 \in \mathbb{N}$ such that

$$\begin{aligned} p_N[T(t)(f_n - f)] &= \sup_{s \in [0, N]} \|f_n(t + s) - f(t + s)\| \\ &\leq \sup_{s \in [0, N+M]} \|f_n(s) - f(s)\| = p_{N+M}[f_n - f] = \epsilon \end{aligned}$$

for all $n \geq n_0$ and $0 \leq t \leq t_0$. That is, even though the shift semigroup is not strongly continuous on $C_b(\mathbb{R}^+, X)$, it is bi-continuous with respect to the topology τ which is coherent with the $\|\cdot\|_\infty$ -topology.

The concept of bi-continuous semigroups on Banach spaces with a coherent locally convex Hausdorff topology τ allows, as in the case of strongly continuous semigroups, a rich qualitative theory. This is due to the fact that key ingredients of the theory of strongly continuous semigroups extend naturally to the bi-continuous case. For example, if

$$Ax := \tau - \lim_{t \rightarrow 0} \frac{T(t)x - x}{t}$$

$$\text{for } x \in D(A) := \{x \in X : \tau - \lim_{t \rightarrow 0} \frac{T(t)x - x}{t} \text{ exists}\},$$

then $T(t)x \in D(A)$, $t \mapsto T(t)x$ is τ -differentiable and

$$\frac{d}{dt}T(t)x = T(t)Ax = AT(t)x$$

for all $t \geq 0$ and $x \in D(A)$. Moreover,

(i) The operator $(A, D(A))$ is bi-closed; i.e., for all sequences $\{x_n\}_{n \in \mathbb{N}}$ in $D(A)$ with $\{x_n\}_{n \in \mathbb{N}}$ and $\{Ax_n\}_{n \in \mathbb{N}}$ $\|\cdot\|$ -bounded, $x_n \xrightarrow{\tau} x \in X$, and $Ax_n \xrightarrow{\tau} y \in X$ we have $x \in D(A)$ and $Ax = y$.

(ii) The domain of the operator A is bi-dense; i.e., for every $x \in X$ there exists a $\|\cdot\|$ -bounded sequence $\{x_n\}$ in $D(A)$ such that $x_n \xrightarrow{\tau} x \in X$

(see Section 1.2 in [37]). Moreover, for all $x \in D(A)$ and $t \geq 0$,

$$T(t)x - x = \tau - \int_0^t T(s)Ax \, ds.$$

If $x \in X$ and $t \geq 0$, then $\tau - \int_0^t T(s)x \, ds \in D(A)$ and

$$T(t)x - x = A(\tau - \int_0^t T(s)x \, ds),$$

where $\tau - \int_0^t T(s)x \, ds$ has to be understood as the τ -Riemann integral

$$\tau - \lim_{\pi \rightarrow 0} \sum T(t'_k)x (t_k - t_{k-1}).$$

We shall now adapt the concept of analytic semigroups in locally convex spaces developed by H. Komatsu in [32] to the bi-continuous case. Let X be a Banach space with a second, coherent topology τ , let $\Sigma_\theta \subset \mathbb{C}$ be a sector of angle $\theta \in (0, \pi]$ and $\{T(z)\}_{z \in \Sigma_\theta \cup \{0\}}$ be a family of bounded linear operators on X . The family $\{T(z)\}_{z \in \Sigma_\theta \cup \{0\}}$ is called a bounded, bi-continuous, analytic semigroup (with respect to a coherent topology τ defined via a family of seminorms \mathcal{P}_τ) if

(i) $T(0) = I$ and $T(z_1 + z_2) = T(z_1)T(z_2)$ for all $z_1, z_2 \in \Sigma_\theta$,

(ii) for all $0 < \theta' < \theta$ there exists $M_{\theta'} \geq 1$ such that $\|T(z)\| \leq M_{\theta'}$ for all $z \in \Sigma_{\theta'}$,

(iii) $\{T(t)\}_{t \geq 0}$ is a bi-continuous semigroup with respect to τ , and

(iv) $z \mapsto \langle T(z)x, x' \rangle$ is analytic on Σ_θ for all $x \in X$ and $x' \in (X, \tau)'$.

It follows from Proposition 8.10 in [32] that bounded, bi-continuous, analytic semigroups are analytic semigroups as defined in Section 9 of [32]. In particular, the complex inversion formula

$$T(t)x = \frac{1}{2\pi i} \int_{\Gamma} e^{\lambda t} R(\lambda, A)x d\lambda \quad (x \in X, t > 0)$$

remains valid, where the integral is in the sense of an improper τ -Riemann integral and the path of integration Γ runs from $\infty e^{-i\omega}$ to $\infty e^{i\omega}$ with $\pi/2 < \omega < \pi/2 + \theta$.

Going back to the shift semigroup (and thus to (1.8)), let $C_b(\bar{\Sigma}_\theta, X)$ denote the space of all bounded continuous functions on a closed sector $\bar{\Sigma}_\theta$ of angle $0 < \theta < \pi/2$. Then

$$\mathcal{X} = F^\infty(\Sigma_\theta, X) := C_b(\bar{\Sigma}_\theta, X) \cap H(\Sigma_\theta, X)$$

equipped with the sup-norm is a Banach space and the (left) shift semigroup $\{T(z)\}_{z \in \Sigma_\theta \cup \{0\}}$ is a bounded, bi-continuous, analytic semigroup on \mathcal{X} (where $T(z)f(\omega) := f(z + \omega)$ for $f \in \mathcal{X}$, $\omega \in \Sigma_\theta$, $z \in \Sigma_\theta$) with respect to the coherent topology τ of uniform convergence on compact subsets of $\bar{\Sigma}_\theta$.

To see this, only property (iv) remains to be shown. For $a \in \bar{\Sigma}_\theta$ and $f \in \mathcal{X}$ define $\mu'_a(f) := f(a)$. Then $\mu'_a \in (\mathcal{X}, \tau)' \subseteq \mathcal{X}^*$ and $N' := \{\mu'_a : a \in \bar{\Sigma}_\theta\}$ is a norming and separating subset of \mathcal{X}^* (and thus of $(\mathcal{X}, \tau)'$). That is,

$$\|f\|_\infty := \sup_{\mu \in N'} |\langle f, \mu \rangle|$$

for all $f \in \mathcal{X}$ and $\langle f, \mu \rangle = 0$ for all $\mu \in N'$ implies $f = 0$.

Since $z \mapsto \langle T(z)f, \mu'_a \rangle = f(z + a)$ is analytic on Σ_θ for all $a \in \bar{\Sigma}_\theta$ (and thus for all $\mu' \in N'$) and since N' is a separating subset of \mathcal{X}^* (and thus of $(\mathcal{X}, \tau)'$), it follows from Theorem A.7 in [2]

that $z \mapsto \langle T(z)f, \varphi \rangle$ is analytic for all $\varphi \in \mathcal{X}^*$ (and thus of $(\mathcal{X}, \tau)'$). Thus the shift semigroup is a bounded, bi-continuous, analytic semigroup on \mathcal{X} .

1.2 Rational Approximations of the Exponential Function

The Hille-Yosida characterization theorem (1.1) states that a densely defined linear operator $(A, D(A))$ generates a strongly continuous semigroup $\{T(t)\}_{t \geq 0}$ with $\|T(t)\| \leq M$ if and only if $\|\lambda^n R(\lambda, A)^n\| \leq M$ for all $\lambda > 0$. Since

$$\lambda R(\lambda, A) = \lambda(\lambda I - A)^{-1} = (I - \frac{1}{\lambda}A)^{-1},$$

this implies for $\lambda = n/t$ ($t > 0, n \in \mathbb{N}$), that the Hille-Yosida condition $\|\lambda^n R(\lambda, A)^n\| \leq M$ for all $\lambda > 0$ is equivalent to

$$\|(I - \frac{t}{n}A)^{-n}\| \leq M \quad t > 0, n \in \mathbb{N}. \quad (1.10)$$

Since

$$\begin{aligned} e^{tz} &= \lim_{n \rightarrow \infty} (1 + \frac{t}{n}z)^n \quad (\text{Forward Euler}), \quad \text{and} \\ e^{tz} &= \lim_{n \rightarrow \infty} (1 - \frac{t}{n}z)^{-n} \quad (\text{Backward Euler}), \end{aligned} \quad (1.11)$$

(1.10) suggests that

$$T(t)x = \lim_{n \rightarrow \infty} (I - \frac{t}{n}A)^{-n}x = \lim_{n \rightarrow \infty} \left(\frac{n}{t} R(\frac{n}{t}, A) \right)^n x. \quad (1.12)$$

The purpose of this section is two-fold. First we summarize some rational approximation results (like (1.10)) for $T(t) = e^{tz}$ ($z \in \mathbb{C}, \operatorname{Re} z \leq 0$); that is, we study rational functions $r(\cdot)$ with the property that $r(\frac{t}{n}z)^n \rightarrow e^{tz}$ ($\operatorname{Re} z \leq 0, t \geq 0$) as $n \rightarrow \infty$. Second, we study the concept of *rational best-approximation* of the exponential function.

Lemma 1.2. *Let $r(\cdot)$ be a differentiable function with $r(0) = 1$ and $r'(0) = 1$. Then $r(\frac{tz}{n})^n \rightarrow e^{tz}$ as $n \rightarrow \infty$ for all $t \in \mathbb{R}$ and $z \in \mathbb{C}$.*

Proof. Since $r(0) = 1$ it follows that $\ln(r(\frac{tz}{n})^n) = n \ln(r(\frac{tz}{n}))$ exists for all n sufficiently large. By L'Hospital's rule,

$$\lim_{n \rightarrow \infty} n \ln(r(\frac{tz}{n})) = \lim_{n \rightarrow \infty} \frac{\ln r(\frac{tz}{n})}{1/n} = \lim_{n \rightarrow \infty} \frac{\frac{1}{r(\frac{tz}{n})} r'(\frac{tz}{n}) \frac{(-tz)}{n^2}}{-1/n^2} = tz.$$

Thus, $r(\frac{tz}{n})^n \rightarrow e^{\ln r(\frac{tz}{n})^n} \rightarrow e^{tz}$. □

In this section our main concern is the question on how to get fast convergence by using appropriate approximating rational functions $r(\cdot)$. In the following, we shall introduce the so called Padé and restricted Padé approximants which appear naturally as the stability functions for implicit Runge-Kutta methods. For details, see [24], [28].

The Euler method is the earliest and simplest numerical approach for solving ordinary differential equations. Consider the initial value problem

$$y'(t) = f(t, y(t)), \quad y(t_0) = y_0.$$

Then the numerical approximation y_1 for the exact solution $y = y(t)$ at $t = t_1 = t_0 + h$, where h is the step-size, is given by

$$y_1 = y_0 + hf(t_0, y(t_0)).$$

As y_1 is directly obtained from y_0 , this is called the explicit(forward) Euler method. The implicit(backward) Euler method is given by the scheme

$$y_1 = y_0 + hf(t_1, y_1),$$

which has to be solved for y_1 given y_0, f and $t_1 = t_0 + h$.

Another frequently used method is the Crank-Nicolson method (also called implicit midpoint rule)

$$y_1 = y_0 + h f(t_0 + \frac{1}{2}h, \frac{1}{2}y_0 + \frac{1}{2}y_1)$$

which, again, has to be solved for y_1 , given y_0, f, t_0 , and h .

Stability functions $z \rightarrow r(z)$ of Runge-Kutta methods can be obtained by using Dahlquist's test problem

$$y'(t) = zy(t), \quad y(0) = y_0, \quad z \in \mathbb{C}, \quad \operatorname{Re}(z) \leq 0.$$

In the case the of backward Euler method,

$$y_1 = y_0 + hf(t_1, y_1) = y_0 + hzy_1$$

or

$$y_1 = \frac{1}{1 - hz} y_0 = r(hz) y_0$$

with $r(z) = \frac{1}{1-z}$.

In the case of Crank-Nicolson method

$$\begin{aligned} y_1 &= y_0 + h f(t_0 + \frac{1}{2}h, \frac{1}{2}y_0 + \frac{1}{2}y_1) \\ &= y_0 + h z (\frac{1}{2}y_0 + \frac{1}{2}y_1) \end{aligned}$$

or

$$y_1 = \frac{2 + hz}{2 - hz} y_0 = r(hz) y_0$$

with

$$r(z) = \frac{2+z}{2-z}. \quad (1.13)$$

Since $y_n = r(hz)^n y_0$, the set $S = \{z \in \mathbb{C} : |r(z)| \leq 1\}$ is called the *stability domain* of the numerical method. Hence, for the backward Euler method, the stability domain is the exterior of the circle centered at 1 with radius 1 and for the Crank-Nicolson method the stability domain is the closed left half-plane $\{z : \operatorname{Re} z \leq 0\}$.

In general, a rational function $r(z) = \frac{P(z)}{Q(z)}$ is called \mathcal{A} -stable if its stability domain contains the closed left half-plane $\{z : \operatorname{Re} z \leq 0\}$. Implicit Runge-Kutta methods whose stability domains include the entire left half plane \mathbb{C}^- are of particular importance since they ensure the stability of the approximation scheme when the exact solution of above Dahlquist's test problem is stable. Other examples of \mathcal{A} -stable stability functions of implicit Runge-Kutta methods are

$$\begin{aligned} \text{(i)} \quad r(z) &= -\frac{6((1+\sqrt{3})z^2 + 2\sqrt{3}z - 6)}{((3+\sqrt{3})z - 6)^2}, \quad \text{Calahan method} \\ \text{(ii)} \quad r(z) &= -\frac{3(z^2 + 8z + 20)}{z^3 - 9z^2 + 36z - 60}, \quad \text{Radau IIA method} \end{aligned}$$

Let $t > 0$ be given and define $h := \frac{t}{n}$ ($n \in \mathbb{N}$, n large). Then $y_n = r(\frac{t}{n}z)^n y_0$ is hoped to be a good approximation to the solution

$$y(t_n) = y(t_0 + n \cdot h) = y(t) = e^{tz} y_0$$

of the Dahlquist's test problem. To investigate the error

$$|y_n - y(t_n)| = |r(\frac{t}{n}z)^n - e^{tz}| |y_0|$$

for \mathcal{A} -stable rational functions $r(\cdot)$ we assume that $r(\cdot)$ is a rational approximation of the exponential function of approximation order $m \geq 1$; i.e., we assume that the first m terms of the Maclaurin expansion of $z \mapsto e^z$ coincide or, equivalently, that

$$|r(z) - e^z| \leq C|z|^{m+1}$$

for $|z|$ sufficiently small.

Lemma 1.3. *If r is an \mathcal{A} -stable rational approximation of the exponential of order $m \geq 1$, then*

$$|r(\frac{t}{n}z)^n - e^{tz}| \leq Ct^{m+1} \frac{1}{n^m} |z|^{m+1} \text{ for } \operatorname{Re}(z) \leq 0 \text{ and } t \geq 0.$$

Proof. By the binomial formula,

$$\begin{aligned} |r(\frac{t}{n}z)^n - e^{tz}| &= |r(\frac{t}{n}z)^n - (e^{\frac{t}{n}z})^n| \\ &= \left| \sum_{j=0}^{n-1} r(\frac{t}{n}z)^{n-1-j} (e^{\frac{t}{n}z})^j \right| \cdot |r(\frac{t}{n}z) - e^{\frac{t}{n}z}| \\ &\leq nC \left| \frac{tz}{n} \right|^{m+1} = Ct^{m+1} \frac{1}{n^m} |z|^{m+1}. \end{aligned}$$

□

A Runge-Kutta method with stability function $r(z) = \frac{P(z)}{Q(z)}$ is \mathcal{A} -stable if and only if $|r(iy)| \leq 1$ and $r(z)$ is analytic for $\operatorname{Re}(z) < 0$. The condition $|r(iy)| \leq 1$ alone means stability on the imaginary axis and is called \mathcal{I} -stability. Since $|r(iy)| \leq 1$ if and only if $\frac{|P(iy)|^2}{|Q(iy)|^2} \leq 1$, it follows that \mathcal{I} -stability is equivalent to the fact that the polynomial

$$E(y) = |Q(iy)|^2 - |P(iy)|^2$$

satisfies $E(y) \geq 0$ for all $y \in \mathbb{R}$.

\mathcal{A} -stability of rational functions and the behavior of exponential function are not wholly consistent as, for example, $e^z \rightarrow 0$ when $|z| \rightarrow \infty$ for $\operatorname{Re}(z) < 0$ while for the stability function $r(z) = \frac{2+z}{2-z}$ of the Crank-Nicolson scheme, we observe $|r(z)| \rightarrow 1$ when $|z| \rightarrow \infty$ for $\operatorname{Re}(z) < 0$. A rational approximation method $r(z)$ is called \mathcal{L} -stable if it is \mathcal{A} -stable and if, in addition,

$$\lim_{z \rightarrow \infty} r(z) = 0.$$

The following proposition is due to Padé and the proof can be found in [45].

Proposition 1.4 (Padé). *If $r(\cdot) = \frac{P(\cdot)}{Q(\cdot)}$ is a rational approximation of the exponential function of approximation order m , then*

$$m \leq \deg(P) + \deg(Q).$$

A rational approximation $r(\cdot) = \frac{P(\cdot)}{Q(\cdot)}$ of maximal approximation order $m = \deg(P) + \deg(Q)$ is called a rational Padé approximation of the exponential. They are of the form

$$\begin{aligned} P(z) &= \sum_{j=0}^{\deg(P)} \frac{(m-j)! \deg(P)!}{j! (\deg(P)-j)!} z^j, \\ Q(z) &= \sum_{j=0}^{\deg(Q)} \frac{(m-j)! \deg(Q)!}{\deg(P)! j! (\deg(Q)-j)!} (-z)^j. \end{aligned} \tag{1.14}$$

The following theorem, whose proof can be found in [24], classifies which Padé approximants are \mathcal{A} -stable and \mathcal{L} -stable, namely, only the first subdiagonal and the second subdiagonal Padé approximations. By first subdiagonal we mean $\deg(Q) - \deg(P) = 1$, and $\deg(Q) - \deg(P) = 2$ for second subdiagonal Padé approximants.

Theorem 1.5. *If $r(\cdot) = \frac{P(\cdot)}{Q(\cdot)}$ is a Padé approximation of the exponential function, then $r(\cdot)$ is \mathcal{A} -stable if and only if*

$$\deg(Q) - 2 \leq \deg(P) \leq \deg(Q).$$

Moreover, the set of all first and second subdiagonal Padé approximations to the exponential function are \mathcal{L} -stable.

It was shown by Ashyralyev and Sobolevskii, [3], that Padé approximations $r(\cdot) = \frac{P(\cdot)}{Q(\cdot)}$ which satisfy $\deg(Q) - 4 \leq \deg(P) \leq \deg(Q)$ have all of their poles in the open right half plane. The following are the widely used first subdiagonal Padé approximations of the exponential function in numerical analysis.

(i) Backward Euler, approximation order $m = 1$,

$$r(z) = \frac{1}{1-z}, \quad \text{pole} = 1$$

(ii) Padé-{1,2} Inversion, approximation order $m = 3$,

$$r(z) = \frac{6+2z}{6-4z+z^2} = \frac{A_1}{b_1-z} + \frac{A_2}{b_2-z}$$

with poles $b_1 = 2 - i\sqrt{2}$, $b_2 = 2 + i\sqrt{2}$, and $A_1 = -1 + i\frac{5\sqrt{2}}{2}$, and $A_2 = -1 - i\frac{5\sqrt{2}}{2}$.

(iii) Radau IIA, approximation order $m = 5$,

$$\begin{aligned} r(z) &= -\frac{3(z^2 + 8z + 20)}{z^3 - 9z^2 + 36z - 60} = \frac{P(z)}{(b_1 - z)(b_2 - z)(b_3 - z)} \\ &= \frac{A_1}{b_1 - z} + \frac{A_2}{b_2 - z} + \frac{A_3}{b_3 - z} \end{aligned}$$

with $A_1 = \frac{P(b_1)}{(b_2 - b_1)(b_3 - b_1)}$, $A_2 = \frac{P(b_2)}{(b_1 - b_2)(b_3 - b_2)}$, $A_3 = \frac{P(b_3)}{(b_1 - b_3)(b_2 - b_3)} = \bar{A}_2$, and poles $b_1 = \{3 - \sqrt[3]{3} + 3^{2/3} (\approx 3.63783)\}$, $b_2 = 3 - \frac{1}{2}3^{2/3} (1 - i\sqrt{3}) + \frac{1}{2}\sqrt[3]{3} (1 + i\sqrt{3}) (\approx 2.68108 + 3.05043i)$, and $b_3 = \bar{b}_2$.

If $r(\cdot) = \frac{r(\cdot)}{Q(\cdot)}$ is a rational Padé approximation to the exponential function, then the zeros of the polynomial $Q(\cdot)$ are distinct, with at most one being real. Now, we shall introduce another class of rational approximations, namely, the *restricted Padé* approximants where the denominator $Q(\cdot)$ is a repeated linear factor.

Rational approximations

$$r_{\{n\}}(z) = \frac{\sum_{j=0}^n (-1)^j L_n^{(n-j)}(1/b) (bz)^j}{(1 - bz)^n} \quad (1.15)$$

are called restricted Padé approximations. Their approximation order is at least n . Here L_n denotes the n th Laguerre polynomial

$$L_n(x) = \sum_{j=0}^n (-1)^j \binom{n}{j} \frac{x^j}{j!}$$

The maximal approximation order m of the restricted Padé approximant $r_{\{n\}}(z)$ is shown to be $m = n + 1$ for suitably picked b . Indeed, there are n different choices of b resulting in the optimal order $m = n + 1$. Details can be found [24], [44]. In connection with our work, we are mainly interested in \mathcal{A} -stable approximations of the exponential. Wanner, Hairer and Nørsette [58] have shown that there is no \mathcal{A} -stable restricted Padé approximation of order greater than 6. Moreover, the \mathcal{A} -stable restricted Padé approximants are precisely $r_{\{1\}}(\cdot)$, $r_{\{2\}}(\cdot)$, $r_{\{3\}}(\cdot)$ and $r_{\{5\}}(\cdot)$.

(i) Crank-Nicolson, approximation order $m = 2$, $r_{\{1\}}(z) = \frac{2+z}{2-z} = -1 + \frac{4}{2-z}$

(ii) Calahan, approximation order $m = 3$,

$$r_{\{2\}}(z) = -\frac{6((1 + \sqrt{3})z^2 + 2\sqrt{3}z - 6)}{((3 + \sqrt{3})z - 6)^2} = B_1 + \frac{B_2}{1 - bz} + \frac{B_3}{(1 - bz)^2}$$

with $b = \frac{1}{6}(3 + \sqrt{3})$, $B_1 = 1 - \sqrt{3}$, $B_2 = -3B_1$, $B_3 = 3 - 2\sqrt{3}$.

(iii) Restricted Padé - Type{3}, order $m = 4$,

$$\begin{aligned} r_{\{3\}}(z) &= \frac{1 - (3b - 1)z - (-3b^2 + 3b - \frac{1}{2})z^2 - (b^3 - 3b^2 + \frac{3}{2}b - \frac{1}{6})z^3}{(1 - bz)^3} \\ &= B_1 + \frac{B_2}{1 - bz} + \frac{B_3}{(1 - bz)^2} + \frac{B_4}{(1 - bz)^3} \end{aligned}$$

$$\text{with } b = \frac{1}{4 - 2 \cos(\frac{\pi}{9}) - 2\sqrt{3} \sin(\frac{\pi}{9})}, B_1 = \frac{6b^3 - 18b^2 + 9b - 1}{6b^3}, B_2 = \frac{12b^2 - 8b + 1}{2b^3}, B_3 = \frac{-8b^2 + 7b - 1}{2b^3}, B_4 = \frac{6b^2 - 6b + 1}{6b^3}$$

(iv) Restricted Padé - Type{5}, order $m = 6$,

$$\begin{aligned} r_{\{5\}}(z) &= \frac{(-b^5 + 5b^4 - 5b^3 + 5b^2 - 5b + 1)z^5 + (5b^4 - 10b^3 + 5b^2 - 5b + 1)z^4}{(1 - bz)^5} \\ &= + \frac{(-10b^3 + 10b^2 - 5b + 1)z^3 + (10b^2 - 5b + 1)z^2 - (5b + 1)z + 1}{(1 - bz)^5} \\ &= B_1 + \frac{B_2}{1 - bz} + \frac{B_3}{(1 - bz)^2} + \frac{B_4}{(1 - bz)^3} + \frac{B_5}{(1 - bz)^4} + \frac{B_6}{(1 - bz)^5} \end{aligned}$$

$$\begin{aligned} \text{with } b \approx 0.47326839, B_1 &= \frac{120b^5 - 600b^4 + 600b^3 - 200b^2 + 25b - 1}{120b^5}, B_2 = \frac{360b^4 - 480b^3 + 180b^2 - 24b + 1}{24b^5}, B_3 = \\ &= \frac{-240b^4 + 390b^3 - 162b^2 + 23b - 1}{12b^5}, B_4 = \frac{180b^4 - 324b^3 + 146b^2 + 22b + 1}{12b^5}, B_5 = \frac{-144b^4 + 276b^3 - 132b^2 + 21b - 1}{24b^5}, B_6 = \\ &= \frac{120b^4 - 240b^3 + 120b^2 - 20b + 1}{120b^5}. \end{aligned}$$

We shall now investigate an alternative way to approximate $t \rightarrow e^{tz}$ for $\text{Re} z \leq 0$ with rational functions $r(z) = \frac{P(z)}{Q(z)}$. To our knowledge, the following 'rational best-approximations' of the exponential function is a new concept. Here is the main idea. We observe first that

$$e^{tz} = \int_0^\infty e^{zs} dH_t(s), \quad \text{Re} z \leq 0, t \geq 0,$$

where $H_t(\cdot)$ is the Heaviside function

$$H_t(s) := \begin{cases} 0 & \text{if } 0 \leq s \leq t, \\ 1 & \text{if } s > t. \end{cases}$$

Now, let $z \rightarrow r(z) = \frac{P(z)}{Q(z)}$ be a rational function with $1 + \deg(P) = \deg(Q) = q$, $r(0) = 1$ and whose poles b_i are all simple with $\operatorname{Re} b_i > 0$ ($1 \leq i \leq q$). Then

$$r(z) = \frac{B_1}{b_1 - z} + \frac{B_2}{b_2 - z} + \dots + \frac{B_q}{b_q - z}$$

with

$$B_i := \frac{P(b_i)}{\prod_{\substack{j=1 \\ j \neq i}}^q (b_j - b_i)}.$$

Let $B \in \mathbb{C}$ and $\operatorname{Re} b > 0$. Then

$$\frac{B}{b - z} = \int_0^\infty e^{zs} d\alpha_{b,B}(s), \quad \operatorname{Re} z \leq 0,$$

for

$$\alpha_{b,B}(s) := \frac{B}{b} [1 - e^{-bs}].$$

In particular,

$$\begin{aligned} r(z) &= \frac{B_1}{b_1 - z} + \frac{B_2}{b_2 - z} + \dots + \frac{B_q}{b_q - z} \\ &= \int_0^\infty e^{zs} d\alpha_r(s) \quad (\operatorname{Re} z \leq 0), \end{aligned}$$

where $\alpha_r(s) = \alpha_{b_1, B_1}(s) + \alpha_{b_2, B_2}(s) + \dots + \alpha_{b_q, B_q}(s)$, and

$$\begin{aligned}
r(z) - e^{tz} &= \int_0^\infty e^{zs} d[\alpha_r(s) - H_t(s)] \quad (\operatorname{Re} z \leq 0, t \geq 0) \\
&= - \int_0^\infty \alpha_r(s) - H_t(s) de^{zs} \\
&= - \int_0^\infty ze^{zs} [\alpha_r(s) - H_t(s)] ds
\end{aligned} \tag{1.16}$$

since $\alpha_r(0) - H_t(0) = 0$, and $\alpha_r(\infty) - H_t(\infty) = \sum_{i=1}^q \frac{B_i}{b_i} - 1 = r(0) - 1 = 0$. In particular

$$|r(z) - e^{tz}| \leq |z| \|\alpha_r - H_t\|_1. \tag{1.17}$$

Thus, we call a rational function

$$r(z) = \frac{B_1}{b_1 - z} + \frac{B_2}{b_2 - z} + \dots + \frac{B_q}{b_q - z}$$

with $r(0) = 1$ and $\operatorname{Re} b_i > 0$ a rational best approximation of degree $(q-1, q)$ of the exponential function at $t \geq 0$ if $\|\alpha_r - H_t\|_1$ is minimal, where

$$\begin{aligned}
\alpha_r(s) &:= \frac{B_1}{b_1} [1 - e^{-b_1 s}] + \frac{B_2}{b_2} [1 - e^{-b_2 s}] + \dots + \frac{B_q}{b_q} [1 - e^{-b_q s}] \\
&= 1 - \frac{B_1}{b_1} e^{-b_1 s} - \frac{B_2}{b_2} e^{-b_2 s} - \dots - \frac{B_q}{b_q} e^{-b_q s} \quad (s \geq 0).
\end{aligned}$$

As a first example, we compute the rational best approximation of degree $(0, 1)$ of the exponential function $t \rightarrow e^{tz}$ ($\operatorname{Re} z \leq 0$) at a given value $t > 0$. That is, we find $r(z) = \frac{B}{b-z}$ with $r(0) = 1$ (or $B = b$) such that $\|\alpha_{(0,1)} - H_t\|_1$ is minimal, where $\alpha_{(0,1)}(s) = \frac{B}{b} [1 - e^{-bs}]$. Now,

$$\begin{aligned}
\|\alpha_{(0,1)} - H_t\|_1 &= \int_0^\infty |\alpha_{(0,1)}(s) - H_t(s)| ds \\
&= \int_0^t |\alpha_{(0,1)}(s)| ds + \int_t^\infty |\alpha_{(0,1)}(s) - 1| ds \\
&= \int_0^t |1 - e^{-bs}| ds + \int_t^\infty e^{-bs} ds \\
&= t + \frac{2}{b}e^{-bt} - \frac{1}{b}
\end{aligned}$$

has a minimum when $(1 + bt)e^{-bt} = 1/2$ or when $b = 1.67835/t$ (MATLAB). In this case,

$$\|\alpha_{(0,1)} - H_t\|_1 = 0.6266t. \quad (1.18)$$

In particular, if $r_t(z) = \frac{1.67835}{1.67835 - tz}$, then $|r_t(z) - e^{tz}| \leq 0.6266t|z|$ for $\operatorname{Re} z \leq 0$.

Similarly, the rational best approximation

$$r(z) = \frac{a + bz}{a - bz} = -b + \frac{a(b+1)}{a-z} \quad (1.19)$$

of degree $(1, 1)$ of the exponential at $t \geq 0$ can be determined. Let $a, b > 0$ and $\operatorname{Re} z \leq 0$. Then

$$\begin{aligned}
|r(z) - e^{tz}| &= \left| \int_0^\infty e^{sz} d[-bH_0(s) + (b+1)[1 - e^{-as}] - H_t(s)] \right| \\
&= \left| - \int_0^\infty z e^{sz} [1 - (1+b)e^{-as} - H_t(s)] ds \right| \\
&\leq |z| \int_0^\infty |1 - (1+b)e^{-as} - H_t(s)| ds \\
&= |z| \left[\int_0^t |1 - (1+b)e^{-as}| ds + \int_t^\infty |(1+b)e^{-as}| ds \right] \\
&= |z| \left[\int_0^{\frac{1}{a} \ln(1+b)} ((1+b)e^{-as} - 1) ds + \int_{\frac{1}{a} \ln(1+b)}^t (1 - (1+b)e^{-as}) ds \right] \\
&\quad + |z| \left[\int_t^\infty (1+b)e^{-as} ds \right] \\
&= |z| \left[t - \frac{2}{a} - \frac{2}{2} \ln(1+b) + \frac{1+b}{a} + \frac{2(1+b)}{a} e^{-at} \right] \\
&= |z| \cdot \|\alpha_{(1,1)} - H_t\|_1,
\end{aligned}$$

where $\alpha_{(1,1)}(s) := 1 - (1+b)e^{-as}$. Using MATLAB we obtain that

$$\|\alpha_{(1,1)} - H_t\|_1 = 0.545816 \cdot t \quad (1.20)$$

if $a = \frac{1.91795}{t}$ and $b = 0.545816$. In particular, if

$$r_t(z) = \frac{1.91795 + 0.545816 \cdot t \cdot z}{1.91795 - tz} = -0.545816 + \frac{2.9648}{t} \cdot \frac{1}{\frac{1.91795}{t} - z},$$

then

$$|r_t(z) - e^{tz}| \leq 0.545816t|z| \quad \text{for } \operatorname{Re} z \leq 0.$$

We now consider rational best-approximations

$$r(z) = \frac{B_1}{b_1 - z} + \frac{B_2}{b_2 - z} \quad (\operatorname{Re} z \leq 0)$$

of degree $(0, 2)$ with $r(0) = \frac{B_1}{b_1} + \frac{B_2}{b_2} = 1$. We remark first that a simple, yet tedious computation shows that the estimate (1.18) can not be improved if b_1 and b_2 are real. Thus, we consider

$$r(z) = \frac{B}{b-z} + \frac{\overline{B}}{\overline{b}-z} \quad (1.21)$$

with $B = B_1 + iB_2$, $b = b_1 + ib_2$ and

$$1 = r(0) = \frac{B}{b} + \frac{\overline{B}}{\overline{b}} = 2\operatorname{Re}\frac{B}{b} = 2 \cdot \frac{B_1b_1 + B_2b_2}{b_1^2 + b_2^2}.$$

In this case, $r(z) = \int_0^\infty e^{sz} d\alpha_{(0,2)}(s)$, where

$$\begin{aligned} \alpha_{(0,2)}(s) &= \frac{B}{b}[1 - e^{-bs}] + \frac{\overline{B}}{\overline{b}}[1 - e^{-\overline{b}s}] = 1 - 2\operatorname{Re}\left[\frac{B}{b}e^{-bs}\right] \\ &= 1 - \frac{2}{b_1^2 + b_2^2}e^{-b_1s}[(B_1b_1 + B_2b_2)\cos b_2s - (B_2b_1 - B_1b_2)\sin b_2s] \\ &= 1 - e^{-b_1s}\left[\cos b_2s - \frac{2(B_2b_1 - B_1b_2)}{b_1^2 + b_2^2}\sin b_2s\right] \\ &= 1 - e^{-b_1s}[\cos b_2s + b_3\sin b_2s] \end{aligned}$$

with $b_3 := \frac{2(-B_2b_1 + B_1b_2)}{b_1^2 + b_2^2}$. Using MATLAB, one obtains that

$$\|\alpha_{(0,2)} - H_t\|_1 = 0.3533 \cdot t \quad (1.22)$$

for $b_1 = 1.9833/t$, $b_2 = 1.619/t$, and $b_3 = 2.4$. Since

$$\begin{aligned} B_1 \cdot b_1 + B_2 \cdot b_2 &= \frac{b_1^2 + b_2^2}{2} \\ B_1 \cdot b_2 - B_2 \cdot b_1 &= 2.4 \cdot \frac{b_1^2 + b_2^2}{2}, \end{aligned}$$

it follows that

$$\begin{aligned}
B_1 &= \frac{1}{2}(b_1 + 2.4b_2) = 6.55464/t, \\
B_2 &= \frac{1}{2}(b_2 - 2.4b_1) = -1.57046/t.
\end{aligned}$$

In particular, if

$$\begin{aligned}
r_t(z) &= \frac{2.93445 - 1.57046i}{1.9833 + 1.619i - tz} + \frac{2.93445 + 1.57046i}{1.9833 - 1.619i - tz} \\
&= \frac{6.55464 - 5.8689tz}{6.55464 - 3.9666tz + t^2z^2},
\end{aligned} \tag{1.23}$$

then

$$|r_t(z) - e^{tz}| \leq 0.3533t \cdot |z| \quad \text{for all } t \geq 0 \text{ and } \operatorname{Re} z \leq 0.$$

We will show in the following section that the inequalities (1.20), (1.22), (1.23) remain valid if z is replaced by a linear operator A generating a bounded, strongly continuous semigroup $T(t) = e^{tA}$ on a Banach space X . For example, it will be shown that for all generators A of strongly continuous semigroups $\{T(t)\}_{t \geq 0}$ satisfying $\|T(t)\| \leq M$ ($t \geq 0$) the inequality (1.20) extends to

$$\left\| \frac{1.67835}{t} R\left(\frac{1.67835}{t}, A\right)x - T(t)x \right\| \leq 0.6266Mt \|Ax\|$$

for all $x \in D(A)$ and $t > 0$.

We now investigate rational best approximations of degree $(q-1, q)$ of the exponential function $t \rightarrow e^{tz}$ assuming that z is in the complement of a sector Σ_θ with $\theta > \pi/2$ (later, in Section 1.3, this will correspond to the case when A generates a bounded analytic semigroup). In this case, we change (1.16) slightly; i.e., we consider

$$\begin{aligned}
r(z) - e^{tz} &= - \int_0^\infty z e^{zs} [\alpha_{(0,1)}(s) - H_t(s)] ds \\
&= \int_0^\infty [-z s e^{zs}] \left[\frac{\alpha_{(0,1)}(s) - H_t(s)}{s} \right] ds.
\end{aligned} \tag{1.24}$$

Since $z = -u + iw$ with $u \geq 0$ and $|w| \leq mu$ it follows that $-z s e^{zs} = (u - iw) s e^{(-u+iw)s}$ or

$$\begin{aligned}
|z s e^{zs}| &= s \sqrt{u^2 + w^2} e^{-us} \leq u s \sqrt{1 + m^2} e^{-us} \\
&\leq e^{-1} \sqrt{1 + m^2} \quad \text{for all } s \geq 0.
\end{aligned}$$

Thus,

$$|r(z) - e^{tz}| \leq e^{-1} \sqrt{1 + m^2} \|g_t(\cdot)\|_1, \tag{1.25}$$

where $g_t(s) = \frac{\alpha_{(0,1)}(s) - H_t(s)}{s}$.

For rational best approximations $r(z) = \frac{b}{b-z}$ of degree $(0, 1)$, the equation (1.25) becomes

$$\begin{aligned}
\left| \frac{b}{b-z} - e^{tz} \right| &\leq C \int_0^\infty \left| \frac{\alpha_{(0,1)}(s) - H_t(s)}{s} \right| ds \\
&= C \left[\int_0^t \frac{1 - e^{-bs}}{s} ds + \int_t^\infty \frac{e^{-bs}}{s} ds \right] \\
&= C \left[\int_0^1 \frac{1 - e^{-ubt}}{u} du + \int_1^\infty \frac{e^{-ubt}}{u} du \right] \\
&=: f(b),
\end{aligned}$$

where $C = e^{-1} \sqrt{1 + m^2}$.

Now,

$$\begin{aligned}
f'(b) &= t \int_0^1 e^{-ubt} du - t \int_1^\infty e^{-ubt} du \\
&= \frac{-1}{b} e^{-ubt} \Big|_0^1 + \frac{1}{b} e^{-ubt} \Big|_1^\infty \\
&= \frac{1}{b} - \frac{2}{b} e^{-bt} = 0
\end{aligned}$$

if $b = \frac{\ln 2}{t}$. Since $f''(b) > 0$, it follows that $f(b)$ is at a minimum if $b = \frac{\ln 2}{t}$. Thus, if $z = -u + iw$ ($u \geq 0, |w| \leq mu$) then

$$\begin{aligned}
\left| \frac{\ln 2}{\ln 2 - tz} - e^{tz} \right| &\leq e^{-1} \sqrt{1 + m^2} \left[\int_0^1 \frac{1 - e^{-u \ln 2}}{u} du + \int_1^\infty \frac{e^{-u \ln 2}}{u} du \right] \\
&\leq 0.968045 \cdot e^{-1} \sqrt{1 + m^2}.
\end{aligned}$$

We will show in the following section that this inequality remains valid if z is replaced by a linear operator A with spectral values $z = -u + iw \in \sigma(A)$ ($u \geq 0, |w| \leq mu$) generating a bounded analytic semigroup $T(t) = e^{tA}$. In this case, we have that

$$\left\| \frac{\ln 2}{t} R\left(\frac{\ln 2}{t}, A\right) - T(t) \right\| \leq 0.968045 \cdot C,$$

where C is such that $\|tAT(t)\| \leq C$.

1.3 Rational Approximations of Operator Semigroups

In this section we shall show how rational approximations of numerical exponential function $t \mapsto e^{tz}$ are used to define rational approximation schemes for operator semigroups $T(t) = e^{tA}$ generated by the operator A . In the analysis of approximation methods, convergence results like the Chernoff Product Formula and the Lax-Richtmyer Equivalence Theorem play an important role in the development of the theory and shall be presented first. Then we shall proceed to approximation results with error estimates due to Hersh and Kato [26] and Brenner and Thomée [7] after briefly

explaining the all important, underlying Hille-Phillips operational calculus. Convergence estimates for bi-continuous semigroups and analytic semigroups will be followed by the stability results due to Hansbo [25] and stabilization techniques obtained by McAllister and Neubrander [42]. Finally, at the end of the section we shall prove rational best approximation results for strongly continuous semigroups.

Let $r(\cdot)$ be a rational approximation of the exponential function and A be the generator of a strongly continuous semigroup $\{T(t)\}_{t \geq 0}$ on some Banach space X . Then the operators $V(t) := r(tA)$, $(t \geq 0)$, are called a rational approximation scheme for $\{T(t)\}_{t \geq 0}$. For example, the backward Euler method $r(z) = \frac{1}{1-z}$ (see (1.11)) and the Crank-Nicolson method $r(z) = \frac{2+z}{2-z}$ (see (1.14)) yield the following operator valued approximation schemes

- Backward Euler, $V_{BE}(t) = r(tA) = (I - tA)^{-1}$,
- Crank-Nicolson $V_{CN}(t) = r(tA) = (I + \frac{t}{2}A)(I - \frac{t}{2}A)^{-1}$.

The following is known as the *Lax-Richtmyer Equivalence Theorem* or *Chernoff Product Formula*. It was shown by Lax and Richtmyer in 1956, [38], under a stronger consistency condition, and in the final form by Chernoff in 1974, [9].

Theorem 1.6. *Suppose that A generates a strongly continuous semigroup $\{T(t)\}_{t \geq 0}$ on a Banach space X and let $\{V(t) : t \geq 0\}$ be an approximation scheme of bounded linear operators with $V(0) = I$ satisfying the consistency condition*

$$\lim_{t \rightarrow 0} \frac{V(t)x - x}{t} = Ax$$

for all $x \in D \subset D(A)$ that is dense in X . Then the following are equivalent:

- (i) $\{V(t)\}_{t \geq 0}$ is stable; that is, there exist $\omega, M \geq 0$ such that $\|V(\frac{t}{n})^n\| \leq Me^{\omega t}$ for each $n \in \mathbb{N}_0$ and $t \geq 0$.

(ii) For all $x \in X$, $V(\frac{t}{n})^n x \rightarrow T(t)x$ ($n \rightarrow \infty$) uniformly for t in compact subsets of \mathbb{R}^+ .

It was shown by Flory [22] that the required consistency condition in the previous theorem is fulfilled for all \mathcal{A} -stable rational approximation schemes. Concordantly, if $r(\cdot)$ is an \mathcal{A} -stable rational approximation of the exponential function of order m and A generates a strongly continuous semigroup, then $V(t) := r(tA)$ is consistent, e.g., $V_{BE}(\cdot)$, $V_{CN}(\cdot)$ are examples of consistent approximation schemes. Notwithstanding of the theoretical importance, the Chernoff Product Formula has two strategic limitations for practical purposes. More specifically, it does not provide any information on the speed of the convergence; i.e., it does not supply any error estimate. Moreover, some of the widely-used consistent approximation schemes become unstable when dealing with non-analytic semigroups; e.g., the Crank-Nicolson scheme is unstable for the shift semigroup (see, for example, [35]). Later in this section we shall cite the stabilization techniques obtained by McAllister and Neubrander [42] for inherently unstable rational approximation methods for strongly continuous semigroups.

In the absence of stability, the crucial convergence results due to Brenner and Thomée [7], based on the earlier work of Hersh and Kato [26], supply the missing particulars on the error estimates and the retrieval of information on the speed of convergence. The fundamental tool for their work is the functional calculus introduced by Hille and Phillips [27]. We choose the alternative approach to the Hille-Phillips calculus through functions of bounded variation obtained by Phillips [47], Kovács [33] instead of the more commonly used approach via regular Borel measures. This preference is not random but due to the fact that the integration by parts formula is naturally valid for functions of bounded variation.

Let $BV[0, a]$ denote the linear space of all complex-valued functions of bounded variation on $[0, a]$. A function $\alpha : [0, a] \rightarrow \mathbb{C}$ is called normalized function of bounded variation, $NBV[0, a]$,

if $\alpha(0) = 0$ and $\alpha(\cdot)$ is right continuous on $(0, a)$, i.e., $\alpha(s) = \frac{\alpha(s+) + \alpha(s-)}{2}$ for all $s \in (0, a)$. Let $V_\alpha(t)$ denote the total variance of α on $[0, t]$. The space

$$NBV := \left\{ \alpha \in \bigcap_{a>0} NBV[0, a] : \sup_{t>0} V_\alpha(t) < \infty \right\}$$

is a commutative Banach algebra with multiplication defined by the *Stieltjes convolution*

$$(\alpha * \beta)(t) := \int_0^t \alpha(t-s) d\beta(s)$$

and norm $\|\alpha\|_{BV} := \sup_{t>0} V_\alpha(t)$. Now, let $\mathbb{C}_0 := \{z \in \mathbb{C} : \operatorname{Re}(z) \leq 0\}$ and $\mathcal{G} := \{f_\alpha : f_\alpha(z) = \int_0^\infty e^{tz} d\alpha(t), z \in \mathbb{C}_0, \alpha \in NBV\}$. The operator $\Phi : NBV \rightarrow \mathcal{G}$ defined by $\Phi(\alpha) := f_\alpha$ is an algebra isomorphism and if we set $\|f_\alpha\| := \|\alpha\|_{BV}$, then \mathcal{G} becomes a Banach algebra. If a rational approximation $r(\cdot)$ is \mathcal{A} -stable, then $r(\cdot) \in \mathcal{G}$. To see this, observe first that $|r(z)| \leq 1$ for $\operatorname{Re} z \leq 0$ implies that all the poles b_i ($1 \leq i \leq q$) are in the right half-plane. Employing partial fractions one obtains

$$r(z) = A_0 + \frac{A_{j_1}}{b_1 - z} + \dots + \frac{A_{j_k}}{(b_1 - z)^k} + \dots + \frac{A_{q_1}}{b_q - z} + \dots + \frac{A_{q_r}}{(b_q - z)^r}$$

for some appropriate constants $A_{i_j} \in \mathbb{C}$. Since the constant functions and the functions $z \mapsto \frac{1}{(b-z)^j}$ ($\operatorname{Re} b > 0$) are in \mathcal{G} ($j \geq 1$) and since \mathcal{G} is an algebra, it follows that $r(\cdot) \in \mathcal{G}$. Now let A generate a strongly continuous semigroup $\{T(t)\}_{t \geq 0}$ with $\|T(t)\| \leq M$ on Banach space X . For $f \in \mathcal{G}$ with $f(z) = \int_0^\infty e^{tz} d\alpha(t)$ ($z \in \mathbb{C}_0$) let

$$f(A)x := \int_0^\infty T(t)x d\alpha(t).$$

Then the Hille-Phillips functional calculus asserts that the map $\Psi : \mathcal{G} \rightarrow \mathcal{B}(X)$ defined by $\Psi(f) := f(A)$ is an algebra homomorphism and $\|f(A)\| \leq M\|\alpha\|_{BV}$. For an extension of the Hille-Phillips functional calculus to bi-continuous semigroups, see [31].

An immediate consequence of the Hille-Phillips functional calculus is the following approximation result.

Theorem 1.7. *Let $(A, D(A))$ be the generator of a bi-continuous semigroup $\{T(t)\}_{t \geq 0}$ on a Banach space X with $\|T(t)\| \leq M$ for all $t \geq 0$. Then, for all $t > 0$ and $x \in D(A)$,*

(i)

$$\left\| \frac{1.67835}{t} R\left(\frac{1.67835}{t}, A\right)x - T(t)x \right\| \leq 0.6266M \cdot t \|Ax\|,$$

(ii)

$$\left\| -0.545816x + \frac{2.9648}{t} R\left(\frac{1.67835}{t}, A\right)x - T(t)x \right\| \leq 0.545816M \cdot t \|Ax\|,$$

(iii)

$$\left\| \frac{B}{t} R\left(\frac{b}{t}, A\right)x + \frac{\bar{B}}{t} R\left(\frac{\bar{b}}{t}, A\right)x - T(t)x \right\| \leq 0.3533M \cdot t \|Ax\|,$$

where $B = 2.93445 - 1.57046i$ and $b = 1.9833 + 1.619i$.

Moreover, if $\{T(t)\}_{t \geq 0}$ is an analytic semigroup with

$$\|tAT(t)\| \leq C$$

for all $t \geq 0$, then

(iv)

$$\left\| \frac{\ln 2}{t} R\left(\frac{\ln 2}{t}, A\right)x - T(t)x \right\| \leq 0.97 \cdot C.$$

Proof. The statements follow from the Hille-Phillips functional calculus in combination with (1.16) - (1.25) □

As we pointed out in Lemma 1.3,

$$\left| r\left(\frac{t}{n}z\right)^n - e^{tz} \right| \leq C t^{m+1} \frac{1}{n^m} |z^{m+1}| \quad \text{for } \operatorname{Re}(z) \leq 0,$$

whenever r is an \mathcal{A} -stable rational approximation of the exponential of order $m \geq 1$. This lemma is the indicator of the linkage between rational approximations of the exponential function and rational approximation schemes for strongly continuous semigroups through the Hille-Phillips functional calculus.

The following theorem from 1979 by Hersh and Kato [26] and in the final form by Brenner and Thomée [7] is one of the key results in the approximation theory for operator semigroups. It shows that Lemma 1.3 remains valid if z is replaced by the generator A of a bounded, strongly continuous semigroup $T(t) = e^{tA}$ on a Banach space X . For an alternative proof, see Kovacs [35] and Kovacs-Neubrandner [36] and for the extension to bi-continuous semigroups, see [31].

Theorem 1.8 (Brenner-Thomée). *Let A generate a bi-continuous semigroup $\{T(t)\}_{t \geq 0}$ with $\|T(t)\| \leq M e^{\omega t}$ for some $M, \omega > 0$. If $V(t) := r(tA)$ for some \mathcal{A} -stable rational approximation r of the exponential of order $m \geq 1$, then $V(\cdot)$ may not be stable. However, there are constants C, κ such that for all $t \geq 0$*

$$\left\| r\left(\frac{t}{n}A\right)^n \right\| \leq CM \sqrt{n} e^{\omega \kappa t}. \quad (1.26)$$

If $k = 0, 1, \dots, m+1$ with $k \neq \frac{m+1}{2}$, then there are $C, c > 0$ (depending only on r) such that

$$\left\| r\left(\frac{t}{n}A\right)^n x - T(t)x \right\| \leq CM e^{c\omega t} t^k \left(\frac{1}{n}\right)^{\beta(k)} \|A^k x\| \quad (1.27)$$

for every $t \geq 0, n \in \mathbb{N}$, and $x \in D(A^k)$, where

$$\beta(k) := \begin{cases} k - \frac{1}{2} & \text{if } 0 \leq k < \frac{m+1}{2}, \\ k \frac{m}{m+1} & \text{if } \frac{m+1}{2} < k \leq m+1. \end{cases}$$

If $k = \frac{m+1}{2}$, then for every $t \geq 0$, $n \in \mathbb{N}$, and $x \in D(A^{\frac{m+1}{2}})$,

$$\|r(\frac{t}{n}A)^n x - T(t)x\| \leq CM e^{c\omega t} t^{\frac{m+1}{2}} \left(\frac{1}{n}\right)^{m/2} \ln(n+1) \|A^{\frac{m+1}{2}} x\|. \quad (1.28)$$

It was shown by Kovacs [34] and Kovacs-Neubrandner [36] that the \ln -term in (1.28) can be dropped if the approximation scheme $\{r(tA)\}_{t \geq 0}$ is stable. Kovacs [34] also has shown that the set of initial data that corresponds to a certain speed of convergence in Theorem 1.8 is not optimal. Indeed, the error estimates given in the theorem extend to initial values in a continuum of intermediate spaces between the Banach space X and the domain of the n -th powers of the generator of the semigroup.

Furthermore, Brenner and Thomée have also shown that the estimate can be improved if \mathcal{A} -stable rational approximation $r(\cdot)$ satisfies the following condition (\star) :

- (a) $|r(is)| < 1$ for $s \in \mathbb{R} - \{0\}$ and $|r(\infty)| < 1$,
- (b) $r(is) = e^{is+\psi(s)}$ with $\psi(s) = O(|s|^{\tilde{q}+1})$ for positive integer \tilde{q} as $s \rightarrow 0$,
- (c) $\operatorname{Re}\psi(s) \leq -\gamma s^{\tilde{p}}$ for $|s| \leq 1$ and some even integer $\tilde{p} \geq \tilde{q} + 1$,

then $\|r(\frac{t}{n}A)^n\| \leq CM n^{(\frac{1}{2} - \frac{\tilde{q}+1}{2\tilde{p}})} e^{\omega \kappa t}$ and above theorem holds with $\beta(k)$ replaced by

$$\beta_*(k) := k \frac{\tilde{q}}{\tilde{q}+1} + \min \left(0, (k - \frac{1}{2}(\tilde{q}+1)) \left(\frac{1}{\tilde{q}+1} - \frac{1}{\tilde{p}} \right) \right).$$

Remarks

- (i) The first subdiagonal Padé approximants $r_{\{j-1,j\}}$ are of order $m = 2j - 1$ and the condition

(\star) holds with $\tilde{p} = 2j$ and $\tilde{q} = 2j - 1$, see [7]. In particular,

$$\|r(\frac{t}{n}A)^n\| \leq CM e^{\omega \kappa t}$$

for all $t \geq 0$ and $\beta_*(k) = k \frac{m}{m+1}$ for $0 \leq k \leq m + 1$, $k \neq j$.

- (ii) The second subdiagonal Padé approximants $r_{\{j-2,j\}}$ are of order $m = 2j - 2$ and the condition $(*)$ holds $\tilde{p} = 2j$ and $\tilde{q} = 2j - 2$, see [7]. In particular,

$$\|r(\frac{t}{n}A)^n\| \leq C_i M n^{1/(4j)} e^{\omega \kappa t}$$

and

$$\beta_*(s) := \begin{cases} s - \frac{2s-1}{2m+4} & \text{if } 0 \leq s < \frac{m+1}{2}, \\ s \frac{m}{m+1} & \text{if } \frac{m+1}{2} < s \leq m+1. \end{cases}$$

- (iii) The restricted Padé approximant $r_{\{2\}}$ (Calahan) has order $m = 3$ and the condition $(*)$ holds with $\tilde{p} = 4$ and $\tilde{q} = 3$. In particular, $r_{\{2\}}(\frac{t}{n}A)^n$ is stable and $\beta_*(k) = \frac{3k}{4}$ (see [7]).

- (iv) The restricted Padé approximant $r_{\{3\}}$ has order $m = 4$ and the condition $(*)$ holds with $\tilde{p} = 6$ and $\tilde{q} = 4$. In particular, $r_{\{3\}}(\frac{t}{n}A)^n$ is $O(n^{1/12})$ and $\beta_*(1) = \frac{3}{4}$ (see [7]).

The Brenner-Thomée estimates bring out several negative messages. First of all, for arbitrary initial data $x \in X$ and without further assumptions on the rational function $r(\cdot)$, Theorem 1.8 forecasts divergence proportional to \sqrt{n} . Also, the theorem predicts on $D(A)$ a speed of convergence of $\frac{1}{n^\beta}$ ($\frac{1}{2} \leq \beta < 1$), regardless of the order of the rational approximation scheme used.

As highlighted earlier, even though the Backward-Euler scheme is stable for generators of strongly continuous semigroups, the other prevalent scheme, Crank-Nicolson is not. However, Ashyralyev and Sobolevskii [3] have proved that the stability result (1.26) in Theorem 1.8 can be generalized to include all first subdiagonal Padé approximations (for an alternative proof of Theorem 1.9. see [50]).

Theorem 1.9 (Ashyralyev - Sobolevskii). *Let X be a Banach space, A be a densely defined operator and $r(\cdot) = \frac{P(\cdot)}{Q(\cdot)}$ be first subdiagonal Padé approximation of the exponential, that is,*

$\deg(P) = \deg(Q) - 1$. Then $r(tA)$ is stable if and only if A generates a strongly continuous semigroup $\{T(t)\}_{t \geq 0}$. In this case,

$$T(t)x = \lim_{n \rightarrow \infty} r\left(\frac{t}{n}A\right)^n x \quad \text{for all } x \in X \quad \text{and } t \geq 0.$$

The absence of stability for certain \mathcal{A} -stable rational approximation schemes for strongly continuous semigroups can be patched up by stabilization methods obtained by Rannacher [49], Hansbo [25], and McAllister and Neubrander [42]. Before furnishing these techniques, we shall first give stability results for the class of analytic semigroups. Indeed, Thomée [55] showed that if A generates an analytic semigroup, then all approximation schemes $V(t) = r(tA)$ defined by \mathcal{A} -stable rational approximations $r(\cdot)$ are stable. The original proofs carry over, almost verbatim, to the bi-continuous, analytic case.

Theorem 1.10. *If A is the generator of a bounded bi-continuous analytic semigroup $\{T(t)\}_{t \geq 0}$ and $r(\cdot)$ is \mathcal{A} -stable rational approximation of the exponential, then there is a constant $C > 0$ satisfying*

$$\|r\left(\frac{t}{n}A\right)^n\| \leq C \text{ for } t \geq 0, n \in \mathbb{N}.$$

There are stronger convergence estimates for \mathcal{A} -stable rational approximations of bounded analytic semigroups as attained by Larsson, Thomée and Wahlbin [40] and Crouzeix, Larsson, Piskarev, and Thomée [11]. Again, the proofs carry over to the bi-continuous case.

Theorem 1.11. *If A is the generator of a bounded bi-continuous analytic semigroup $\{T(t)\}_{t \geq 0}$ and $r(\cdot)$ is \mathcal{A} -stable rational approximation of the exponential of approximation order m , then there is a constant C satisfying*

$$\|r\left(\frac{t}{n}A\right)^n x - T(t)x\| \leq CM \left(\frac{t}{n}\right)^m \|A^m x\| \text{ for } t \geq 0, x \in D(A^m)$$

Theorem 1.12. *If A is the generator of a bounded bi-continuous analytic semigroup $\{T(t)\}_{t \geq 0}$ and $r(\cdot)$ is \mathcal{A} -stable rational approximation of the exponential of approximation order m with $|r(\infty)| < 1$, then there is a constant $C > 0$ such that, for $t \geq 0$,*

$$\|r(\frac{t}{n}A)^n - T(t)\| \leq CM \frac{1}{n^m}.$$

Though \mathcal{A} -stable rational approximations r are stable for analytic semigroups $\{T(t)\}_{t \geq 0}$ generated by A , the convergence $r(\frac{t}{n}A)^n x \rightarrow T(t)x$ can be arbitrarily slow for non-smooth initial data if $\|r(\infty)\| = 1$ (e.g., Crank-Nicolson). Rannacher [49], and in the final form Hansbo [25], proposed a stabilization technique for unstable rational approximations by first applying a stable lower order approximation with $\|r(\infty)\| = 0$ and then combining the smoothing property of the lower order scheme with the improved accuracy of the higher order approximation scheme. In the following, $s(A)$ stands for the spectral bound of the operator A ; i.e., $s(A) := \sup\{\operatorname{Re}(\lambda) : \lambda \in \sigma(A)\}$.

Theorem 1.13 (Hansbo). *Let $(A, D(A))$ be an operator on a Banach space X . Suppose that $s(A) < 0$ and that $(A, D(A))$ generates an analytic semigroup $T(\cdot)$ on X with $s(A) < 0$. Let $r_a(\cdot)$ be an \mathcal{A} -stable rational approximation of the exponential of approximation order $m \geq 2$ and $r_s(\cdot)$ is \mathcal{A} -stable and of order $m - 1$ with $r_s(\infty) = 0$. Define*

$$r_n(z) := \begin{cases} r_s(z)^n & \text{if } n < m, \\ r_a(z)^{n-m} r_s(z)^m & \text{if } n \geq m, \end{cases}$$

Then,

$$\|r_n(\frac{t}{n}A)x - T(t)x\| \leq C \frac{1}{n^m} \|x\| \quad \text{for all } x \in X.$$

For example, to stabilize the Crank-Nicolson scheme, one would apply two steps of the Backward-Euler scheme first.

Hansbo uses the classic Dunford-Riesz functional calculus for analytic semigroups in the proof of the above theorem. That is,

$$f(A) := \frac{1}{2\pi i} \int_{\Gamma} f(\lambda) R(\lambda, A) d\lambda,$$

where Γ is the boundary of a sector $\Sigma_{\theta} := \{\lambda : |\arg(\lambda)| < \frac{\pi}{2} + \theta\}$ for some $\theta \in (0, \frac{\pi}{2}]$ that is contained in the resolvent set of A and where f is analytic on an open neighborhood of the complement of Σ_{θ} . In particular, the spectrum of A must be contained in a sector $\{\lambda : |\arg(-\lambda)| \leq \alpha\}$ for some $\alpha \in (0, \frac{\pi}{2})$. Thus, the methods of Hansbo are not applicable for non-analytic semigroups.

The stabilization of rational approximation schemes for non-analytic strongly continuous semigroups was investigated by McAllister and Neubrander. For the proofs of the following results see [42].

Theorem 1.14. *Let A be the generator of a strongly continuous semigroup $\{T(t)\}_{t \geq 0}$ on a Banach space X . Define $V(t) := r(tA)$, where $r(\cdot)$ is an \mathcal{A} -stable rational approximation of the exponential of approximation order m and a stabilizing scheme*

$$W(t) := \frac{1}{t^{\alpha}} R\left(\frac{1}{t^{\alpha}}, A\right) = (I - t^{\alpha} A)^{-1},$$

where $\alpha = \frac{m}{m+2}$. Then, for all $\tau > 0$ there exists a constant M_{τ} such that

$$\|V\left(\frac{t}{n}\right)^n W\left(\frac{t}{n}\right)^{m+1} x - T(t)x\| \leq 2M_{\tau} \left(\frac{1}{n}\right)^{\frac{m}{m+2}} (\|x\| + \|Ax\|)$$

for all $t \in [0, \tau]$, all $x \in D(A)$, and all sufficiently large $n \geq m + 1$. Furthermore,

$$\lim_{n \rightarrow \infty} V\left(\frac{t}{n}\right)^n W\left(\frac{t}{n}\right)^{m+1} x = T(t)x$$

for all $x \in X$.

Theorem 1.15. *Let A be the generator of a strongly continuous semigroup $\{T(t)\}_{t \geq 0}$ on a Banach space X . Define $V(t) := r(tA)$, where $r(\cdot)$ is an \mathcal{A} -stable rational approximation of the exponential of approximation order m and define a stabilizing scheme $W(\cdot)$:*

$$W(t) = \sum_{i=1}^k \frac{a_i}{t^\alpha} R\left(\frac{b_i}{t^\alpha}, A\right),$$

where $0 < b_1 < b_2 < \dots < b_{k-1} < b_k$ are arbitrarily chosen, $\alpha := \frac{m}{m+k+1}$, and

$$a_i := \frac{(-1)^{k+i} b_i^k}{\prod_{\substack{j=1 \\ j \neq i}}^k |b_j - b_i|}.$$

So that $W(t)$ can be represented in the form

$$W(t) := (-1)^{k+1} t^{k\alpha} A^k \prod_{i=1}^k (b_i I - t^\alpha A)^{-1} + I.$$

Then

$$\lim_{n \rightarrow \infty} V\left(\frac{t}{n}\right)^n W\left(\frac{t}{n}\right)^{m+1} x = T(t)x$$

for all $x \in X$. Furthermore, for all $\tau > 0$ there exists a constant M_τ such that

$$\left\| V\left(\frac{t}{n}\right)^n W\left(\frac{t}{n}\right)^{m+1} x - T(t)x \right\| \leq 2M_\tau \left(\frac{1}{n}\right)^{\frac{km}{m+k+1}} (\|x\| + \|A^k x\|)$$

for all $t \in [0, \tau]$, all $x \in D(A^k)$, and all sufficiently large $n \geq m + 1$.

Proposition 1.16. *Let A be the generator of a strongly continuous semigroup $\{T(t)\}_{t \geq 0}$ and let $V(t) := r(tA)$, where r is an \mathcal{A} -stable rational approximation of the exponential of approximation order m . Define*

$$W(t) := \frac{1}{\sqrt{t}} R\left(\frac{1}{\sqrt{t}}, A\right) = \left(I - \frac{1}{\sqrt{t}} A\right)^{-1}.$$

Then

$$\lim_{n \rightarrow \infty} V\left(\frac{t}{n}\right)^{n-1} W\left(\frac{t}{n}\right) = T(t)x$$

for all $x \in X$ uniformly on compact intervals.

Chapter 2

Numerical Inversion of the Laplace Transform

In this chapter we shall introduce a set of entirely new, numerically and analytically effective and efficient inversion formulas for the Laplace transform. Our methods are obtained by applying the Hersh-Kato [26] and Brenner-Thomée [7] results on \mathcal{A} -stable rational approximations of operator semigroups to the (left) shift semigroup for operator-valued functions. Since the results hold for Banach space valued functions, our *rational inversion* techniques turn out to be an adequate tool to study time-discretization procedures for convolution-type evolution equations (e.g., linear first order and higher order abstract Cauchy problems, inhomogeneous abstract Cauchy problems, delay equations, Volterra and integro-differential equations, etc.). In Sections 2.2 and 2.3 we shall give illustrations of rational Laplace transform inversions. In particular, we shall give detailed discussions of subdiagonal and restricted Padé inversions of the Laplace transforms. Finally, in Section 2.4, we apply the results to the inhomogeneous abstract Cauchy problem.

2.1 Rational Inversion of the Laplace Transform

In this section we introduce a new class of Laplace transform inversion procedures that come with sharp error estimates yielding wellposedness of the inversion in appropriate norms. In contrast to Talbot's method for the numerical inversion of the Laplace transform (see [1], [39], [53], [59], [60]), the rational Laplace transform inversions do not require the analyticity of the Laplace transform for $\lambda \in \mathbb{C}$ with $\frac{\pi}{2} \leq |\arg(\lambda)| < \frac{\pi}{2} + \epsilon$ and $|\lambda| > r$ ($\epsilon, r > 0$). Our inversion procedures are, therefore, applicable to parabolic and hyperbolic problems alike. The inversion methods are derived from the theory of rational approximation methods for strongly continuous operator semigroups using results due to Hersh and Kato [26], Brenner and Thomée [7], Larsson, Thomée and Wahlbin [40], Hansbo [25], and Crouzeix, Larsson, Piskarev and Thomée [11].

As discussed earlier, the papers [7], [11], [26], and [40] contain some of the main results for rational approximation schemes $V(t) := r(tA)$ for strongly continuous operator semigroups $\{T(t)\}_{t \geq 0}$ generated by a linear operator A with domain $D(A)$ and range in a Banach space X , where $r = \frac{P}{Q}$ (P, Q polynomials with $p = \deg(P) \leq \deg(Q) = q$) is an \mathcal{A} -stable rational approximation of the exponential function of order m .

We have shown in Lemma 1.3 that if r is an \mathcal{A} -stable rational approximation of the exponential of order $m \geq 1$, then $|r(\frac{t}{n}z)^n - e^{tz}| \leq Ct^{m+1} \frac{1}{n^m} |z|^{m+1}$ for $\operatorname{Re}(z) \leq 0$ and $t \geq 0$. It is one of the key results in the approximation theory for operator semigroups (see Theorem 1.8) that Lemma 1.3 holds if z is replaced by the generator A of a bounded, strongly continuous semigroup $T(t) = e^{tA}$ on a Banach space X ; i.e.,

$$\|r(\frac{t}{n}A)^n x - e^{tA}x\| \leq \tilde{C}t^{m+1} \frac{1}{n^m} \|A^{m+1}x\| \quad (2.1)$$

for all $x \in D(A^{m+1})$. Moreover, if r is an \mathcal{A} -stable approximation of the exponential, then $r(\frac{t}{n}A)^n x - e^{tA}x \rightarrow 0$ for all $x \in X$ (uniformly for t in compact in if and only if the operators $V(t) := r(tA)$ are stable; that is, there exist $\omega, M \geq 0$ such that $\|V(\frac{t}{n})^n\| \leq Me^{\omega t}$ for each $n \in \mathbb{N}_0$ and $t \geq 0$. This follows from Theorem 1.6.

Approximation schemes $V(t) = r(tA)$ defined by \mathcal{A} -stable rational approximation r of the exponential of order $m \geq 1$ were investigated in the ground-breaking papers of Hersh and Kato [26] and Brenner and Thomée [7]. The rational inversion formula for the Laplace transform and the error estimates we shall discuss in this section are an immediate consequence of Theorem 1.8. As we highlighted earlier, there are stronger convergence estimates for \mathcal{A} -stable rational approximations of bounded analytic semigroups as attained by Larsson, Thomée and Wahlbin [40] and Crouzeix, Larsson, Piskarev, and Thomée [11], Theorems 1.11, 1.12. In the following, we shall show that Theorems 1.8, 1.11, 1.12 yield sharp inversion methods for the Laplace transform by applying

them to the shift semigroup $T(t)u : s \rightarrow u(t+s)$ with generator $A = d/ds$ on spaces \mathcal{X} of continuous functions (where we always take A with its maximal domain $D(A) = \{u \in \mathcal{X} : u' \in \mathcal{X}\}$.) The results below will confirm that the seemingly simple advection equation

$$w_t(t, s) = w_s(t, s), w(0, s) = u(s), t, s \geq 0 \quad (2.2)$$

is, from a numerical point of view, already one of the most revealing linear partial differential equations. It will be shown, that the advection equation is not only a suitable test case for numerical methods for approximations of hyperbolic problems (see also [8], [18], [56]), but for all convolution type evolution equations. That is, numerical results for the shift semigroup translate into results for the Laplace transform, and thus to all problems that can be treated with Laplace transform techniques. The following results concerning the shift semigroup are needed.

Let X be a Banach space. We denote by $\mathcal{C}_b(\mathbb{R}^+, X)$ the Banach space of bounded and continuous functions from \mathbb{R}^+ into X and $\mathcal{C}_0(\mathbb{R}^+, X) := \{u \in \mathcal{C}_b(\mathbb{R}^+, X) : u(\infty) = 0\}$. Let Σ_θ be the sector $\{z \in \mathbb{C} \setminus \{0\} : |\arg(z)| < \theta\}$, $H(\Sigma_\theta, X)$ the space of all analytic functions $u : \Sigma_\theta \rightarrow X$, and $C_{ub}(\overline{\Sigma_\theta}, X)$ the space of all bounded, uniformly continuous functions from Σ_θ into X . The shift semigroup is strongly continuous on $\mathcal{C}_0(\mathbb{R}^+, X)$, bi-continuous on $\mathcal{C}_b(\mathbb{R}^+, X)$, bounded, strongly continuous and analytic on $C_{ub}(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X)$ (see [4], [30]), and bounded, bi-continuous, and analytic on $C_b(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X)$.

Let X be a Banach space. Consider the shift semigroup $T(t)u : s \rightarrow u(t+s)$ on $\mathcal{X} = \mathcal{C}_0(\mathbb{R}^+, X)$ (or $\mathcal{C}_b(\mathbb{R}^+, X)$ or $C_b(\overline{\Sigma_\theta}, X)$). Then, $T(t)_{t \geq 0}$ is a strongly continuous (bi-continuous, analytic) semigroup with generator $A = d/ds$, where $D(A) = \{u \in \mathcal{X} : u' \in \mathcal{X}\}$. Since

$$R(\lambda, A)u = \int_0^\infty e^{-\lambda t} T(t)u \, dt = \int_0^\infty e^{-\lambda t} u(t + \cdot) \, dt,$$

it follows that

$$R(\lambda, A)u(0) = \int_0^\infty e^{-\lambda t} u(t) dt = \hat{u}(\lambda)$$

(the Laplace transform of u). Consequently,

$$\begin{aligned} R(\lambda, A)^{n+1}u(0) &= \frac{(-1)^n}{n!} R(\lambda, A)^{(n)}u(0) \\ &= \frac{(-1)^n}{n!} \int_0^\infty e^{-\lambda t} (-t)^n u(t) dt = \frac{(-1)^n}{n!} \hat{u}^{(n)}(\lambda). \end{aligned}$$

Now, let $r(z) = \frac{P(z)}{Q(z)}$ be an \mathcal{A} -stable rational approximation to the exponential function of order $m \geq 1$. Then, using partial fraction decomposition, there exist constants $B_0, B_{\{1,i,j\}}, b_i \in \mathbb{C}$ with $\operatorname{Re}(b_i) > 0$, and $r_i \in \mathbb{N}$ such that

$$r(z) = B_0 + \sum_{i=1}^s \sum_{j=1}^{r_i} \frac{B_{\{1,i,j\}}}{(b_i - z)^j},$$

or, more general, for each $n \in \mathbb{N}$, there exist constants $B_{\{n,i,j\}} \in \mathbb{C}$ such that

$$r^n(z) = B_0^n + \sum_{i=1}^s \sum_{j=1}^{nr_i} \frac{B_{\{n,i,j\}}}{(b_i - z)^j}. \quad (2.3)$$

(see Section 2.2 and Section 2.3). In particular,

$$\begin{aligned} r^n \left(\frac{t}{n} A \right) u(0) &= B_0^n u(0) + \sum_{i=1}^s \sum_{j=1}^{nr_i} B_{\{n,i,j\}} R \left(b_i, \frac{t}{n} A \right)^j u(0) \\ &= B_0^n u(0) + \sum_{i=1}^s \sum_{j=1}^{nr_i} B_{\{n,i,j\}} \left(\frac{n}{t} \right)^j R \left(\frac{nb_i}{t}, A \right)^j u(0) \\ &= B_0^n u_0 + \sum_{i=1}^s \sum_{j=1}^{nr_i} B_{\{n,i,j\}} \left(\frac{n}{t} \right)^j \frac{(-1)^{j-1}}{(j-1)!} \hat{u}^{(j-1)} \left(\frac{nb_i}{t} \right), \end{aligned}$$

where $u_0 := \lim_{\lambda \rightarrow \infty} \lambda \hat{u}(\lambda) = u(0)$. Since

$$T(t)u(0) = u(t),$$

it follows that the approximation error

$$\begin{aligned} E(n, t, u) : &= \left\| B_0^n u_0 + \sum_{i=1}^s \sum_{j=1}^{nr_i} B_{\{n,i,j\}} \left(\frac{n}{t}\right)^j \frac{(-1)^{j-1}}{(j-1)!} \hat{u}^{(j-1)} \left(\frac{nb_i}{t}\right) - u(t) \right\|_X \\ &= \left\| r^n \left(\frac{t}{n} A\right) u(0) - u(t) \right\|_X = \left\| r^n \left(\frac{t}{n} A\right) u(0) - T(t)u(0) \right\|_X \end{aligned}$$

can be estimated by

$$E(n, t, u) \leq \left\| r^n \left(\frac{t}{n} A\right) u - T(t)u \right\|_\infty. \quad (2.4)$$

Thus, the semigroup results of Theorems (1.8), (1.11), (1.12) yield the following statements concerning the inversion of the Laplace transform.

Theorem 2.1 (Rational Laplace Transform Inversion). *Let $u \in \mathcal{X} = \mathcal{C}_0(\mathbb{R}^+, X)$ (or $\mathcal{C}_b(\mathbb{R}^+, X)$ or $\mathcal{C}_b(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X)$) and let r be an \mathcal{A} -stable rational approximation of the exponential function of order $m \geq 1$ with constants $B_0, B_{\{1,i,j\}}, b_i \in \mathbb{C}, r_i \in \mathbb{N}$ as defined in (2.3). Let $u_0 := \lim_{\lambda \rightarrow \infty} \lambda \hat{u}(\lambda) = u(0)$ and consider the error term*

$$E(n, t, u) := \left\| B_0^n u_0 + \sum_{i=1}^s \sum_{j=1}^{nr_i} B_{\{n,i,j\}} \left(\frac{n}{t}\right)^j \frac{(-1)^{j-1}}{(j-1)!} \hat{u}^{(j-1)} \left(\frac{nb_i}{t}\right) - u(t) \right\|_X.$$

Then the following statements hold.

(i) *If $|r(\infty)| < 1$ and $u \in \mathcal{C}_b(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X)$, then for all $t \geq 0$,*

$$E(n, t, u) \leq C \frac{1}{n^m} \|u\|_\infty.$$

Moreover, by using Hansbo's Theorem 1.13, the approximation scheme can be stabilized so that the error term $\tilde{E}(n, t, u)$ of the the modified scheme satisfies

$$\tilde{E}(n, t, u) \leq C \frac{1}{n^m} \|u\|_\infty.$$

for all $u \in C_b(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X)$.

(ii) If $|r(\infty)| = 1$ and $u, u^{(m)} \in C_b(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X)$, then for all $t \geq 0$,

$$E(n, t, u) \leq Ct^m \frac{1}{n^m} \|u^{(m)}\|_\infty.$$

(iii) If $u, u^{(k)} \in C_b(\mathbb{R}^+, X)$ for some $1 \leq k \leq m+1$, then for all $t \geq 0$,

$$E(n, t, u) \leq Ct^k \frac{1}{n^{\gamma(k)}} \|u^{(k)}\|_\infty,$$

where $\gamma(k)$ is given by $\beta(k)$ or $\beta_*(k)$ as defined in Theorem 1.8. In particular,

$$E(n, t, u) \leq \begin{cases} Ct^{m+1} \frac{1}{n^m} \|u^{(m+1)}\|_\infty & \text{if } u, u^{(m+1)} \in C_b(\mathbb{R}^+, X), \\ Ct^{\frac{1}{n^\beta}} \|u^{(1)}\|_\infty & \text{if } u, u^{(1)} \in C_b(\mathbb{R}^+, X), \end{cases}$$

for all $t \geq 0$, where $\beta \in [\frac{1}{2}, 1)$ is given by $\beta(1)$ or $\beta_*(1)$ as defined in Theorem 1.8.

(iv) If $V(t) := r(tA)$ is stable for $A = d/ds$ on one of the spaces $\mathcal{X} = C_0(\mathbb{R}^+, X)$ (or $C_b(\mathbb{R}^+, X)$) then for all $u \in \mathcal{X}$ and $t \geq 0$,

$$\lim_{n \rightarrow \infty} E(n, t, u) = 0$$

If $V(t) = r(tA)$ is not stable, then the stabilization Theorems 1.14-1.16 allow to stabilize the scheme so that

- (a) the error term $\tilde{E}(n, t, u)$ of the modified scheme satisfies $\tilde{E}(n, t, u) \rightarrow 0$ as $n \rightarrow \infty$ for all $u \in C_0(\mathbb{R}^+, X)$, and
- (b) the order of convergence can be improved slightly for $f \in C_0^1([0, \infty), X)$.

2.2 Subdiagonal Padé Inversion of the Laplace Transform

To provide a first example of rational Laplace transform inversion procedures, consider the subdiagonal Padé approximants $r_{\{s-1, s\}} := r$ with $r(z) = \frac{P(z)}{Q(z)}$, where P, Q are as in (1.14). These Padé approximants are \mathcal{A} -stable, of order $m = 2s - 1$, and the statements of Theorem (1.12) and the item (c) in (\star) condition for Theorem (1.8) hold. It is known (see, e.g., [24], [51]) that r has s distinct poles b_i with $\operatorname{Re}(b_i) > 0$. Thus, using partial fraction decomposition,

$$r(z) = \sum_{j=1}^s \frac{B_j}{b_j - z}, \quad (2.5)$$

where

$$B_j = \frac{P(b_j)}{\prod_{i \neq j} (b_i - b_j)}.$$

To see this, let

$$r(z) = \frac{a_0 + a_1 z + \dots + a_{s-1} z^{s-1}}{(b_1 - z)(b_2 - z) \dots (b_s - z)} := \frac{P(z)}{(b_1 - z)(b_2 - z) \dots (b_s - z)}.$$

Then,

$$r(z) = \frac{P(z)}{(b_1 - z)(b_2 - z) \dots (b_s - z)} = \frac{B_1}{b_1 - z} + \frac{B_2}{b_2 - z} + \dots + \frac{B_s}{b_s - z},$$

where $B_j = \frac{P(b_j)}{\prod_{i \neq j} (b_i - b_j)}$ if and only if

$$P(z) = B_1(b_2 - z)(b_3 - z) \dots (b_s - z) + \dots + B_s(b_1 - z)(b_2 - z) \dots (b_{s-1} - z)$$

Then, for $z = b_1$, we have; $P(b_1) = B_1(b_2 - b_1)(b_3 - b_1) \dots (b_s - b_1)$. Thus, $B_1 = \frac{P(b_1)}{(b_2 - b_1)(b_3 - b_1) \dots (b_s - b_1)}$.

For $z = b_2$, we have; $P(b_2) = B_2(b_1 - b_2)(b_3 - b_2) \dots (b_s - b_2)$. Thus, $B_2 = \frac{P(b_2)}{(b_1 - b_2)(b_3 - b_2) \dots (b_s - b_2)}$.

Hence, it follows that

$$B_j = \frac{P(b_j)}{\prod_{i \neq j} (b_i - b_j)}.$$

Before giving the complete partial fraction formula for $r(z)^n$ for an arbitrary power n in Lemma 2.4, we shall first give details for the cases when $n = 2$ and $n = 3$. These cases will be of special importance when using rational approximation methods with high approximation order m .

Lemma 2.2. Let $r(z) = \frac{a_0 + a_1 z + \dots + a_{s-1} z^{s-1}}{(b_1 - z)(b_2 - z) \dots (b_s - z)}$, then

$$r(z)^2 = \frac{B_{11}}{b_1 - z} + \frac{B_{12}}{(b_1 - z)^2} + \dots + \frac{B_{s1}}{b_s - z} + \frac{B_{s2}}{(b_s - z)^2},$$

where

$$B_{i1} = 2B_i \sum_{\substack{k=1 \\ k \neq i}}^s \frac{B_k}{b_k - b_i} \quad \text{and} \quad B_{i2} = B_i^2$$

and B_i 's are as defined above.

Proof. Let $r(z) = \frac{B_1}{b_1 - z} + \frac{B_2}{b_2 - z} + \dots + \frac{B_s}{b_s - z}$. Then,

$$\begin{aligned} r(z)^2 &= \left(\frac{B_1}{b_1 - z} + \frac{B_2}{b_2 - z} + \dots + \frac{B_s}{b_s - z} \right)^2 \\ &= \sum_{i=1}^s \frac{B_i^2}{(b_i - z)^2} + \sum_{i=1}^{s-1} \sum_{j=i+1}^s \frac{2B_i B_j}{(b_i - z)(b_j - z)}. \end{aligned}$$

Since for any i, j ,

$$\frac{2B_i B_j}{(b_i - z)(b_j - z)} = \frac{2B_i B_j}{(b_i - z)(b_j - b_i)} + \frac{2B_i B_j}{(b_j - z)(b_i - b_j)},$$

we have

$$\frac{B_{i1}}{b_i - z} = \frac{2B_i}{b_i - z} \sum_{\substack{k=1 \\ k \neq i}}^s \frac{B_k}{b_k - b_i}.$$

Therefore,

$$B_{i1} = 2B_i \sum_{\substack{k=1 \\ k \neq i}}^s \frac{B_k}{b_k - b_i} \quad \text{and} \quad B_{i2} = B_i^2,$$

as desired. □

Lemma 2.3. *Let $r(z) = \frac{a_0 + a_1 z + \dots + a_{s-1} z^{s-1}}{(b_1 - z)(b_2 - z) \dots (b_s - z)}$, then*

$$r(z)^3 = \sum_{i=1}^s \frac{C_{i1}}{b_i - z} + \sum_{i=1}^s \frac{C_{i2}}{(b_i - z)^2} + \sum_{i=1}^s \frac{C_{i3}}{(b_i - z)^3}$$

where

$$C_{i1} = 2B_i \left(\sum_{\substack{j=1 \\ j \neq i}}^s \sum_{\substack{k=1 \\ k \neq i}}^s \frac{B_j B_k}{(b_j - b_i)(b_k - b_i)} + \frac{B_j B_k}{(b_j - b_k)(b_k - b_i)} \right) + B_i \sum_{\substack{j=1 \\ j \neq i}}^s \frac{B_j^2}{(b_i - b_j)^2} \\ - B_i^2 \sum_{\substack{j=1 \\ j \neq i}}^s \frac{B_j}{(b_j - b_i)^2}$$

$$C_{i2} = 3B_i^2 \sum_{\substack{j=1 \\ j \neq i}}^s \frac{B_j}{b_j - b_i}$$

$$C_{i3} = B_i^3,$$

and where the B_i 's are as in previous lemma.

Proof. Let $r(z) = \frac{B_1}{b_1-z} + \frac{B_2}{b_2-z} + \dots + \frac{B_s}{b_s-z}$. Then,

$$\begin{aligned}
r(z)^3 &= \left(\frac{B_1}{b_1-z} + \frac{B_2}{b_2-z} + \dots + \frac{B_s}{b_s-z} \right)^2 \cdot \left(\frac{B_1}{b_1-z} + \frac{B_2}{b_2-z} + \dots + \frac{B_s}{b_s-z} \right) \\
&= \left(\sum_{i=1}^s \frac{B_{i1}}{b_i-z} + \sum_{i=1}^s \frac{B_i^2}{(b_i-z)^2} \right) \cdot \left(\frac{B_1}{b_1-z} + \frac{B_2}{b_2-z} + \dots + \frac{B_s}{b_s-z} \right) \\
&= \sum_{i=1}^s \sum_{\substack{j=1 \\ j \neq i}}^s \frac{B_{i1}B_j}{(b_i-z)(b_j-z)} + \sum_{i=1}^s \frac{B_{i1}B_i}{(b_i-z)^2} + \sum_{i=1}^s \sum_{\substack{j=1 \\ j \neq i}}^s \frac{B_i^2B_j}{(b_i-z)^2(b_j-z)} \\
&\quad + \sum_{i=1}^s \frac{B_i^3}{(b_i-z)^3}
\end{aligned}$$

Now,

$$\begin{aligned}
\sum_{i=1}^s \sum_{\substack{j=1 \\ j \neq i}}^s \frac{B_i^2B_j}{(b_i-z)^2(b_j-z)} &= \sum_{i=1}^s \sum_{\substack{j=1 \\ j \neq i}}^s \frac{B_i^2B_j}{b_i-b_j} \cdot \frac{1}{(b_i-z)^2} + \sum_{i=1}^s \sum_{\substack{j=1 \\ j \neq i}}^s \frac{B_i^2B_j}{(b_i-b_j)^2} \cdot \frac{1}{b_j-z} \\
&\quad - \sum_{i=1}^s \sum_{\substack{j=1 \\ j \neq i}}^s \frac{B_i^2B_j}{(b_i-b_j)^2} \cdot \frac{1}{b_i-z}
\end{aligned}$$

and,

$$\sum_{i=1}^s \frac{B_{i1}B_i}{(b_i-z)^2} = \sum_{i=1}^s \sum_{\substack{j=1 \\ j \neq i}}^s \frac{2B_i^2B_j}{b_i-b_j} \cdot \frac{1}{(b_i-z)^2}.$$

Thus,

$$\begin{aligned}
\sum_{i=1}^s \sum_{\substack{j=1 \\ j \neq i}}^s \frac{B_{i1}B_j}{(b_i-z)(b_j-z)} &= \sum_{i=1}^s \sum_{\substack{j=1 \\ j \neq i}}^s \frac{B_{i1}B_j}{b_j-b_i} \cdot \frac{1}{b_i-z} - \sum_{i=1}^s \sum_{\substack{j=1 \\ j \neq i}}^s \frac{B_{i1}B_j}{b_j-b_i} \cdot \frac{1}{b_j-z} \\
&= \sum_{i=1}^s \sum_{\substack{j=1 \\ j \neq i}}^s \sum_{\substack{k=1 \\ k \neq i}}^s \left(\frac{2B_iB_jB_k}{(b_j-b_i)(b_k-b_i)} + \frac{2B_iB_jB_k}{(b_j-b_k)(b_k-b_i)} \right) \cdot \frac{1}{b_i-z}
\end{aligned}$$

as desired. □

Lemma 2.4. *If a rational function is of the form (2.5), then for each $n \in \mathbb{N}$,*

$$r(z)^n = \sum_{i=1}^s \sum_{j=1}^n \frac{B_{\{n,i,j\}}}{(b_i - z)^j}, \quad (2.6)$$

where the constants $B_{\{n,i,k\}}$ ($1 \leq i \leq s, 1 \leq k \leq n$) are inductively given by

$$\begin{aligned} B_{\{n+1,i,1\}} &= \sum_{k=1}^n \sum_{\substack{j=1 \\ j \neq i}}^s a_{ij}^k [(-1)^{k+1} B_{\{n,i,k\}} \cdot B_{\{1,j,1\}} + B_{\{n,j,k\}} \cdot B_{\{1,i,1\}}] \\ B_{\{n+1,i,n+1\}} &= B_{\{n,i,n\}} \cdot B_{\{1,i,1\}} \\ B_{\{n+1,i,r\}} &= \left[\sum_{k=r}^n \sum_{\substack{j=1 \\ j \neq i}}^s B_{\{n,i,k\}} \cdot B_{\{1,j,1\}} \cdot a_{ij}^{k-r+1} \cdot (-1)^{k-r} \right] \\ &+ B_{\{n,i,r-1\}} \cdot B_{\{1,i,1\}} \quad \text{for all } 2 \leq r \leq n, \end{aligned}$$

and $a_{ij} := \frac{1}{b_j - b_i}$.

For the proof, see [31]. Thus, for a subdiagonal Padé approximation r of the exponential function of order $m = 2s - 1$ ($s \geq 1$) with given poles b_1, b_2, \dots, b_s , Theorem 2.1 is applicable with $B_0 = 0$ and $B_{\{n,i,j\}}$ given as above. Observe that (i) and (iv) of Theorem 2.1 are applicable since $r(\infty) = 0$ and $r(tA)$ is stable for $A = d/ds$ on all spaces \mathcal{X} of continuous functions considered above. For $s = 1, 2, 3, 4$ (respectively $m = 1, 3, 5, 7$) the subdiagonal Padé Inversions of the Laplace transform are as follows.

m=1: Backward Euler Inversion (Post-Widder). If $s = 1$ then $m = 1$ and the subdiagonal Padé approximation $r_{\{0,1\}}$ (Backward Euler) is given by

$$r(z) = \frac{1}{1 - z}.$$

Since $r(z)^n = \frac{1}{(1-z)^n}$, (2.3) holds with $s = 1$, $r_1 = 1$, $b_1 = 1$, $B_0 = 0$, $B_{\{n,1,n\}} = 1$, and $B_{\{n,1,j\}} = 0$ for $j \neq n$. Thus, Theorem 2.1 holds for $m = 1$ and

$$E_{be}(n, t, u) := \left\| \frac{(-1)^{n-1}}{(n-1)!} \left(\frac{n}{t}\right)^n \widehat{u}^{(n-1)} \left(\frac{n}{t}\right) - u(t) \right\|_X \quad (2.7)$$

satisfies, for all $t \geq 0$,

$$E_{be}(n, t, u) \leq \begin{cases} Ct \frac{1}{\sqrt{n}} \|u^{(1)}\|_\infty & \text{if } u, u^{(1)} \in \mathcal{C}_b(\mathbb{R}^+, X) \\ Ct^2 \frac{1}{n} \|u^{(2)}\|_\infty & \text{if } u, u^{(2)} \in \mathcal{C}_b(\mathbb{R}^+, X), \\ C \frac{1}{n} \|u\|_\infty & \text{if } u \in C_b(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X). \end{cases}$$

Moreover, $\lim_{n \rightarrow \infty} E_{be}(n, t, u) = 0$ for all $u \in \mathcal{C}_b(\mathbb{R}^+, X)$ and the Backward Euler approximations (2.7) retain essential structural characteristics of u (positivity, monotonicity, convexity, etc.; see [29], [35]). To see the connection between (2.7) and the Post-Widder inversion

$$\frac{(-1)^n}{n!} \left(\frac{n}{t}\right)^{n+1} \widehat{u}^{(n)} \left(\frac{n}{t}\right), \quad (2.8)$$

define $U(t) := \int_0^t u(r) dr$ and $\hat{U}(\lambda) := \int_0^\infty e^{-\lambda t} U(t) dt$. Since $\hat{U}(\lambda) = \frac{1}{\lambda} \hat{u}(\lambda)$ it follows that

$$\begin{aligned} \frac{(-1)^{n-1}}{(n-1)!} \left(\frac{n}{t}\right)^n \widehat{U}^{(n-1)} \left(\frac{n}{t}\right) &= \sum_{j=0}^{n-1} \frac{(-1)^j}{j!} \left(\frac{n}{t}\right)^j \widehat{u}^{(j)} \left(\frac{n}{t}\right) \\ &= \int_0^t \frac{(-1)^n}{n!} \left(\frac{n}{s}\right)^{n+1} \widehat{u}^{(n)} \left(\frac{n}{s}\right) ds. \end{aligned}$$

By applying (2.7) to U and \hat{U} and by using (1.8) in [20], it follows that

$$E_{be}(n, t, U) := \left\| \int_0^t \frac{(-1)^n}{n!} \left(\frac{n}{s}\right)^{n+1} \widehat{u}^{(n)} \left(\frac{n}{s}\right) ds - \int_0^t u(s) ds \right\|_X \leq 2t \frac{1}{\sqrt{n}} \|u\|_\infty.$$

Thus, for all $u \in \mathcal{C}_b(\mathbb{R}^+, X)$, the Post-Widder inversion (2.8) converges "in the average" towards u at a rate of $\frac{1}{\sqrt{n}}$ (see also [21]). It is well known (see, e.g., Thm 1.7.7 in [2]) that the Post-Widder

inversion (2.8) converges pointwise to $u(t)$ for all $u \in \mathcal{C}_{b,\omega}(\mathbb{R}^+, X)$ and all $t \geq 0$; however, the convergence can be arbitrarily slow.

m=3: Padé-{1,2} Inversion. If $s = 2$ then $m = 3$ and the subdiagonal Padé approximation $r_{\{1,2\}}$ is given by

$$r(z) = \frac{6 + 2z}{6 - 4z + z^2} = \sum_{i=1}^2 \frac{B_{\{1,i,1\}}}{b_i - z},$$

where $b_{1,2} = 2 \pm i\sqrt{2}$, $B_{\{1,1,1\}} = -1 + i\frac{5\sqrt{2}}{2}$, and $B_{\{1,2,1\}} = -1 - i\frac{5\sqrt{2}}{2}$. Now (2.3) holds for $B_0 = 0$, $r_i = 1$, and $B_{\{n,i,j\}}$ to be computed as in (2.6) with $s = 2$. It follows that Theorem 2.1 holds for $m = 3$ and that

$$E(n, t, u) := \left\| \sum_{i=1}^2 \sum_{j=1}^n B_{\{n,i,j\}} \left(\frac{n}{t}\right)^j \frac{(-1)^{j-1}}{(j-1)!} \hat{u}^{(j-1)} \left(\frac{nb_i}{t}\right) - u(t) \right\|_X \quad (2.9)$$

satisfies

$$E(n, t, u) \leq \begin{cases} Ct^k \frac{1}{n^{3k/4}} \|u^{(k)}\|_\infty & \text{if } u, u^{(k)} \in \mathcal{C}_b(\mathbb{R}^+, X) \text{ and } 1 \leq k \leq 4, \\ C \frac{1}{n^3} \|u\|_\infty & \text{if } u \in C_b(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X) \end{cases}$$

for all $t \geq 0$. Moreover, $\lim_{n \rightarrow \infty} E(n, t, u) = 0$ for all $u \in \mathcal{C}_b(\mathbb{R}^+, X)$.

m=5: Radau IIA Inversion. If $s = 3$ then $m = 5$ and the subdiagonal Padé approximant $r_{\{2,3\}}$ is given by

$$r(z) = \frac{3z^2 + 24z + 60}{-z^3 + 9z^2 - 36z + 60} = \sum_{i=1}^3 \frac{B_{\{1,i,1\}}}{b_i - z},$$

where $b_1 = 3 - 3^{1/3} + 3^{2/3} \approx 3.63$, $b_{2,3} = 3 - \frac{1}{2}3^{2/3} + \frac{1}{2}3^{1/3} \pm \frac{1}{2}i(3^{5/6} + 3^{7/6}) \approx 2.68 \pm 3.05i$ and $B_{\{1,i,1\}} = \frac{60 + 24b_i + 3b_i^2}{\prod_{k \neq i} (b_k - b_i)}$. Now (2.3) holds for $B_0 = 0$, $r_i = 1$, and $B_{\{n,i,j\}}$ to be computed as in (2.6) with $s = 3$. It follows that Theorem 2.1 holds for $m = 5$ and that

$$E(n, t, u) := \left\| \sum_{i=1}^3 \sum_{j=1}^n B_{\{n,i,j\}} \left(\frac{n}{t}\right)^j \frac{(-1)^{j-1}}{(j-1)!} \widehat{u}^{(j-1)} \left(\frac{nb_i}{t}\right) - u(t) \right\|_X \quad (2.10)$$

satisfies

$$E(n, t, u) \leq \begin{cases} Ct^{\frac{1}{n^{5k/6}}} \|u^{(k)}\|_{\infty} & \text{if } u, u^{(k)} \in \mathcal{C}_b(\mathbb{R}^+, X) \text{ and } 1 \leq k \leq 6, \\ C \frac{1}{n^5} \|u\|_{\infty} & \text{if } u \in C_b(\overline{\Sigma_{\theta}}, X) \cap H(\Sigma_{\theta}, X) \end{cases}$$

for all $t \geq 0$. Moreover, for all $u \in \mathcal{C}_b(\mathbb{R}^+, X)$, $\lim_{n \rightarrow \infty} E(n, t, u) = 0$.

m=7: Padé-{3,4} Inversion. The largest value of s for which all constants can be computed symbolically is $s = 4$. Then $m = 7$ and the subdiagonal Padé approximation $r_{\{3,4\}}$ is given by

$$r(z) = \frac{4z^3 + 60z^2 + 360z + 840}{z^4 - 16z^3 + 120z^2 - 480z + 840} = \sum_{i=1}^4 \frac{B_{\{1,i,1\}}}{b_i - z},$$

where

$$\begin{aligned} b_{1,2} &= 4 - \sqrt{-4 + \frac{10^{2/3}}{\sqrt[3]{-2 + i\sqrt{6}}} + \sqrt[3]{10(-2 + i\sqrt{6})}} \\ &\pm \sqrt{-8 - \frac{10^{2/3}}{\sqrt[3]{-2 + i\sqrt{6}}} - \sqrt[3]{10(-2 + i\sqrt{6})} - \frac{8}{\sqrt{-4 + \frac{10^{2/3}}{\sqrt[3]{-2 + i\sqrt{6}}} + \sqrt[3]{10(-2 + i\sqrt{6})}}}} \\ &\approx 3.212 \pm 4.773i \end{aligned}$$

$$\begin{aligned} b_{3,4} &= 4 + \sqrt{-4 + \frac{10^{2/3}}{\sqrt[3]{-2 + i\sqrt{6}}} + \sqrt[3]{10(-2 + i\sqrt{6})}} \\ &\pm \sqrt{-8 - \frac{10^{2/3}}{\sqrt[3]{-2 + i\sqrt{6}}} - \sqrt[3]{10(-2 + i\sqrt{6})} + \frac{8}{\sqrt{-4 + \frac{10^{2/3}}{\sqrt[3]{-2 + i\sqrt{6}}} + \sqrt[3]{10(-2 + i\sqrt{6})}}}} \\ &\approx 4.787 \pm 1.567i \end{aligned}$$

and $B_{\{1,i,1\}} = \frac{4b_i^3 + 60b_i^2 + 360b_i + 84}{\prod_{k \neq i} (b_k - b_i)}$. Now (2.3) holds for $B_0 = 0$, $r_i = 1$, and $B_{\{n,i,j\}}$ to be computed as in (2.6) with $s = 3$. It follows that Theorem 2.1 holds for $m = 7$ and that

$$E(n, t, u) := \left\| \sum_{i=1}^4 \sum_{j=1}^n B_{\{n,i,j\}} \left(\frac{n}{t} \right)^j \frac{(-1)^{j-1}}{(j-1)!} \widehat{u}^{(j-1)} \left(\frac{nb_i}{t} \right) - u(t) \right\|_X \quad (2.11)$$

satisfies for all $t \geq 0$

$$E(n, t, u) \leq \begin{cases} Ct^k \frac{1}{n^{7k/8}} \|u^{(k)}\|_\infty & \text{if } u, u^{(k)} \in \mathcal{C}_b(\mathbb{R}^+, X) \text{ and } 1 \leq k \leq 8, \\ C \frac{1}{n^7} \|u\|_\infty & \text{if } u \in C_b(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X). \end{cases}$$

Moreover, for all $u \in \mathcal{C}_b(\mathbb{R}^+, X)$, $\lim_{n \rightarrow \infty} E(n, t, u) = 0$.

Since the poles of r are given symbolically, all $4n$ coefficients $B_{\{n,i,j\}}$ ($1 \leq i \leq 4, 1 \leq j \leq n$) needed in (2.11) are, in principal, computable symbolically (error free). However, since in applications it is often difficult to handle $\widehat{u}^{(j-1)}$ for large j (i.e., $j \geq 3$), let us consider (2.11) for $n = 2$. In this case, the eight coefficients $B_{\{2,i,j\}}$ ($1 \leq i \leq 4, 1 \leq j \leq 2$) are easily computable

$$B_{\{2,i,1\}} = \sum_{\substack{j=1 \\ j \neq i}}^4 \frac{2B_{\{1,i,1\}}B_{\{1,j,1\}}}{b_j - b_i}, \quad B_{\{2,i,2\}} = B_{\{1,i,1\}}^2,$$

and the 8-term inversion

$$E(2, t, u) := \left\| \sum_{i=1}^4 \sum_{j=1}^2 B_{\{2,i,j\}} \left(\frac{2}{t} \right)^j \frac{(-1)^{j-1}}{(j-1)!} \widehat{u}^{(j-1)} \left(\frac{2b_i}{t} \right) - u(t) \right\|_X. \quad (2.12)$$

gives already reasonable results since $1/2^7 = 0.0078125$. In order to get better approximations while keeping the number of derivatives low, one has to increase the order m .

m=21: Padé-{10,11} Inversion. If $s = 11$ then $m = 21$ and the subdiagonal Padé approximation $r_{\{10,11\}}$ is given by

$$r(z) = \frac{P(z)}{Q(z)} = \sum_{i=1}^{11} \frac{B_{\{1,i,1\}}}{b_i - z},$$

where P with $\deg(P) = 10$ and Q with $\deg(Q) = 11$ are as in (1.14) and where the zeros b_i of Q are given by $b_{1,2} \approx 5.46 \pm 17.60i, b_{3,4} \approx 9.23 \pm 13.71i, b_{5,6} \approx 11.60 \pm 10.15i, b_{7,8} \approx$

$13.11 \pm 6.72i$, $b_{9,10} \approx 13.96 \pm 3.34i$, $b_{11} \approx 14.23$, and $B_{\{1,i,1\}} = \frac{P(b_i)}{\prod_{k \neq i} (b_k - b_i)}$. For $n = 2$, the 22 coefficients $B_{\{2,i,j\}}$ ($1 \leq i \leq 11, 1 \leq j \leq 2$) can be computed to any degree of accuracy and are given by

$$B_{\{2,i,1\}} = \sum_{\substack{j=1 \\ j \neq i}}^{11} \frac{2B_{\{1,i,1\}}B_{\{1,j,1\}}}{b_j - b_i}, \text{ and } B_{\{2,i,2\}} = B_{\{1,i,1\}}^2.$$

Consider the 22-term inversion

$$E(2, t, u) := \left\| \sum_{i=1}^{11} \sum_{j=1}^2 B_{\{2,i,j\}} \left(\frac{2}{t} \right)^j \frac{(-1)^{j-1}}{(j-1)!} \hat{u}^{(j-1)} \left(\frac{2b_i}{t} \right) - u(t) \right\|_X. \quad (2.13)$$

Since $1/2^{21} \leq 0.0000005$, Theorem 2.1 gives reasonable good results for $n = 2$ since

$$E(2, t, u) \leq \begin{cases} Ct^k \frac{1}{2^{21k/22}} \|u^{(k)}\|_\infty & \text{if } u, u^{(k)} \in \mathcal{C}_b(\mathbb{R}^+, X) \text{ and } 1 \leq k \leq 22, \\ C \frac{1}{2^{21}} \|u\|_\infty & \text{if } u \in C_b(\overline{\Sigma}_\theta, X) \cap H(\Sigma_\theta, X). \end{cases}$$

Clearly, the choice of $m = 21$ was arbitrary; i.e., if $n = 2$ and the subdiagonal Padé inversion should have an approximation error $E(n, t, u)$ of order 10^{-N} , then m should be an odd number larger than $10N/3$.

2.3 Restricted Padé Inversion of the Laplace Transform

To provide a second class of examples of rational Laplace transform inversions, consider the \mathcal{A} -stable restricted Padé approximants $r_{\{1\}}$ (Crank-Nicolson, $m = 2$) and $r_{\{2\}}$ (Calahan, $m = 3$), where $r_{\{j\}}$ is defined as in (1.15). In contrast to the subdiagonal Padé approximants with $m > 1$, these approximants have only one single real pole. Therefore, their associated Laplace transform inversions require only the knowledge of $\hat{u}(\lambda)$ for real $\lambda > 0$.

m=2: Crank-Nicolson Inversion. The Crank-Nicolson approximation

$$r(z) = \frac{2+z}{2-z} = -1 + \frac{4}{2-z}$$

is an \mathcal{A} -stable Padé approximation of the exponential function of order $m = 2$.

Let $u_0 = \lim_{\lambda \rightarrow \infty} \lambda \hat{u}(\lambda) = u(0)$. Since

$$r\left(\frac{t}{n}z\right)^n = \sum_{j=0}^n \binom{n}{j} (-1)^{n-j} 2^{2j} \left(\frac{n}{t}\right)^j \frac{1}{\left(\frac{2n}{t} - z\right)^j},$$

it follows from Theorem 2.1 that

$$E(n, t, u) := \left\| (-1)^n u_0 + (-1)^{n-1} \sum_{j=1}^n \binom{n}{j} 4^j \left(\frac{n}{t}\right)^j \frac{1}{(j-1)!} \hat{u}^{(j-1)}\left(\frac{2n}{t}\right) - u(t) \right\|_{\mathbb{X}}$$

satisfies, for all $t \geq 0$,

$$E(n, t, u) \leq \begin{cases} Ct \frac{1}{\sqrt{n}} \|u^{(1)}\|_{\infty} & \text{if } u, u^{(1)} \in \mathcal{C}_b(\mathbb{R}^+, X), \\ Ct^k \frac{1}{n^{2k/3}} \|u^{(k)}\|_{\infty} & \text{if } u, u^{(k)} \in \mathcal{C}_b(\mathbb{R}^+, X) \text{ and } 2 \leq k \leq 3, \\ Ct^2 \frac{1}{n^2} \|u^{(2)}\|_{\infty} & \text{if } u, u^{(2)} \in C_b(\overline{\Sigma_{\theta}}, X) \cap H(\Sigma_{\theta}, X). \end{cases}$$

For $u \in C_{ub}(\overline{\Sigma_{\theta}}, X) \cap H(\Sigma_{\theta}, X)$ the results can be improved by using Hansbo's stabilization methods [25]; for $u, u^{(1)} \in \mathcal{C}_b(\mathbb{R}^+, X)$ the results can be improved by stabilizing the Crank-Nicolson scheme using the methods in [42].

For example, stabilizing the Crank-Nicolson scheme with the Hansbo's method, we have to compute

$$\begin{aligned} r_{CN}(z)^{n-2} r_{BE}(z)^2 &= \left(-1 + \frac{4}{2-z}\right)^{n-2} \left(\frac{1}{1-z}\right)^2 \\ &= \sum_{j=0}^{n-2} 2^{2j} (-1)^{n-j} \left[\frac{1}{(2-z)^j} \frac{1}{(1-z)^2} \right]. \end{aligned}$$

An easy induction shows that

$$\frac{1}{(2-z)^j} \frac{1}{(1-z)} = \frac{1}{1-z} - \sum_{i=1}^j \frac{1}{(2-z)^i}.$$

Thus

$$\begin{aligned}
\frac{1}{(2-z)^j} \frac{1}{(1-z)^2} &= \frac{1}{(1-z)^2} - \sum_{i=1}^j \frac{1}{(2-z)^i} \frac{1}{(1-z)} \\
&= \frac{1}{(1-z)^2} - \sum_{i=1}^j \left[\frac{1}{1-z} - \sum_{m=1}^i \frac{1}{(2-z)^m} \right] \\
&= \frac{1}{(1-z)^2} - \frac{j}{1-z} + \sum_{m=1}^j \frac{j-m+1}{(2-z)^m}.
\end{aligned}$$

It follows that

$$\begin{aligned}
r_{CN}(z)^{n-2} r_{BE}(z)^2 &= \sum_{j=0}^{n-2} \binom{n-2}{j} 2^{2j} (-1)^{n-j} \left[\frac{1}{(1-z)^2} - \frac{j}{1-z} + \sum_{m=1}^j \frac{j-m+1}{(2-z)^m} \right] \\
&= \frac{3^{n-2}}{(1-z)^2} + \frac{(n-2)3^{n-3} \cdot 4}{1-z} + \sum_{j=0}^{n-2} \binom{n-2}{j} 2^{2j} (-1)^{n-j} \frac{j-m+1}{(2-z)^m}.
\end{aligned}$$

Since

$$r(z) = (-1 + \frac{4}{2-z})^{n-2} = \sum_{j=0}^{n-2} \binom{n-2}{j} 2^{2j} (-1)^{n-j} \frac{1}{(2-z)^j}$$

and

$$r'(z) = (n-2)(-1 + \frac{4}{2-z})^{n-3} \frac{4}{(2-z)^2} = \sum_{j=0}^{n-2} \binom{n-2}{j} 2^{2j} (-1)^{n-j} \frac{j}{(2-z)^{j+1}}$$

it follows that

$$r(1) = 3^{n-2} = \sum_{j=0}^{n-2} \binom{n-2}{j} 2^{2j} (-1)^{n-j}$$

and

$$r'(1) = (n-2)3^{n-3} \cdot 4 = \sum_{j=0}^{n-2} \binom{n-2}{j} 2^{2j} (-1)^{n-j} \cdot j.$$

Thus

$$\begin{aligned}
r_{CN}(z)^{n-2} r_{BE}(z)^2 &= \frac{3^{n-2}}{(1-z)^2} + \frac{(n-2)3^{n-3} \cdot 4}{1-z} + \sum_{m=1}^{n-2} \sum_{j=m}^{n-2} \binom{n-2}{j} 2^{2j} (-1)^{n-j} \frac{j-m+1}{(2-z)^m} \\
&= \frac{3^{n-2}}{(1-z)^2} + \frac{(n-2)3^{n-3} \cdot 4}{1-z} + \sum_{m=1}^{n-2} \frac{B_{m,n}}{(2-z)^m},
\end{aligned}$$

where

$$B_{m,n} = \sum_{j=m}^{n-2} \binom{n-2}{j} 2^{2j} (-1)^{n-j} (j-m+1).$$

Since

$$r_{CN}\left(\frac{t}{n}z\right)^{n-2} r_{BE}\left(\frac{t}{n}z\right)^2 = \left(\frac{n}{t}\right)^2 \frac{3^{n-2}}{\left(\frac{n}{t}z - z\right)^2} + \left(\frac{n}{t}\right) \frac{(n-2)3^{n-3} \cdot 4}{\frac{n}{t}z - z} + \sum_{m=1}^{n-2} \left(\frac{2n}{t}\right)^m \frac{B_{m,n}}{\left(\frac{2n}{t}z - z\right)^m},$$

it follows from Theorem 2.1 that $E_{\text{stabilized}}(n, t, u) :=$

$$\left\| -\left(\frac{n}{t}\right)^2 3^{n-2} \hat{u}^{(1)}\left(\frac{n}{t}\right) + \left(\frac{n}{t}\right) (n-2) 3^{n-3} \cdot 4 \hat{u}\left(\frac{n}{t}\right) + \sum_{m=1}^{n-2} \left(\frac{2n}{t}\right)^m \frac{(-1)^{m-1}}{(m-1)!} B_{m,n} \hat{u}^{(m-1)}\left(\frac{2n}{t}\right) - u(t) \right\|$$

satisfies, for all $t \geq 0$,

$$E_{\text{stabilized}}(n, t, u) \leq \frac{C}{n^2} \|u\|_{\infty}$$

if $u \in C_{ub}(\overline{\Sigma_{\theta}}, X) \cap H(\Sigma_{\theta}, X)$.

m=3: Calahan Inversion. The Calahan approximation

$$r(z) = B_1 + \frac{B_2}{1-bz} + \frac{B_3}{(1-bz)^2}$$

with $b = \frac{1}{6}(3 + \sqrt{3})$, $B_1 = 1 - \sqrt{3}$, $B_2 = 3(-1 + \sqrt{3})$, $B_3 = 3 - 2\sqrt{3}$ is an \mathcal{A} -stable restricted Padé approximation of e^z of order $m = 3$. Since

$$r\left(\frac{t}{n}z\right)^n = \sum_{j=0}^n \sum_{k=0}^j \binom{n}{j} B_1^{n-j} B_2^{j-k} B_3^k \binom{j}{k} \left(\frac{n}{bt}\right)^{k+j} \frac{1}{\left(\frac{n}{bt} - z\right)^{k+j}},$$

it follows from Theorem 2.1 that $E(n, t, u) :=$

$$\left\| B_1^n u_0 + \sum_{j=1}^n \sum_{k=0}^j \binom{n}{j} \binom{j}{k} B_1^{n-j} B_2^{j-k} B_3^k \left(\frac{n}{bt}\right)^{j+k} \frac{(-1)^{j+k-1}}{(j+k-1)!} \widehat{u}^{(j+k-1)}\left(\frac{n}{bt}\right) - u(t) \right\|_X$$

satisfies

$$E(n, t, u) \leq \begin{cases} Ct^k \frac{1}{n^{3k/4}} \|u^{(k)}\|_\infty & \text{if } u, u^{(k)} \in \mathcal{C}_b(\mathbb{R}^+, X) \text{ and } 1 \leq k \leq 4, \\ C \frac{t^3}{n^3} \|u^{(3)}\|_\infty & \text{if } u, u^{(3)} \in C_b(\overline{\Sigma}_\theta, X) \cap H(\Sigma_\theta, X) \end{cases}$$

for all $t \geq 0$. Moreover, the stability of the Calahan scheme (see Theorem 1.8, Remark (iii)) implies that $\lim_{n \rightarrow \infty} E(n, t, u) = 0$ for all $u \in \mathcal{C}_b(\mathbb{R}^+, X)$.

m=4, Restricted Padé - Type{3}. The rational approximation $r_{\{3\}}$

$$\begin{aligned} r(z) &= \frac{1 - (3b - 1)z - (-3b^2 + 3b - \frac{1}{2})z^2 - (b^3 - 3b^2 + \frac{3}{2}b - \frac{1}{6})z^3}{(1 - bz)^3} \\ &= B_1 + \frac{B_2}{1 - bz} + \frac{B_3}{(1 - bz)^2} + \frac{B_4}{(1 - bz)^3} \end{aligned}$$

with $b = \frac{1}{4 - 2 \cos(\frac{\pi}{9}) - 2\sqrt{3} \sin(\frac{\pi}{9})}$, $B_1 = \frac{6b^3 - 18b^2 + 9b - 1}{6b^3}$, $B_2 = \frac{12b^2 - 8b + 1}{2b^3}$, $B_3 = \frac{-8b^2 + 7b - 1}{2b^3}$, $B_4 = \frac{6b^2 - 6b + 1}{6b^3}$ is an \mathcal{A} -stable restricted Padé approximation of e^z of order $m = 4$.

Since

$$\begin{aligned}
r(z)^n &= \left(B_1 + \frac{B_2}{1-bz} + \frac{B_3}{(1-bz)^2} + \frac{B_4}{(1-bz)^3} \right)^n \\
&= \sum_{j=0}^n \binom{n}{j} B_1^{n-j} \left(\frac{B_2}{1-bz} + \frac{B_3}{(1-bz)^2} + \frac{B_4}{(1-bz)^3} \right)^j \\
&= \sum_{j=0}^n \binom{n}{j} B_1^{n-j} \frac{1}{(1-bz)^j} \left(B_2 + \frac{B_3}{1-bz} + \frac{B_4}{(1-bz)^2} \right)^j \\
&= \sum_{j=0}^n \binom{n}{j} B_1^{n-j} \frac{1}{(1-bz)^j} \left(\sum_{k=0}^j \binom{j}{k} B_2^{j-k} \left(\frac{B_3}{1-bz} + \frac{B_4}{(1-bz)^2} \right)^k \right) \\
&= \sum_{j=0}^n \sum_{k=0}^j \binom{n}{j} \binom{j}{k} B_1^{n-j} B_2^{j-k} \frac{1}{(1-bz)^{j+k}} \left(\sum_{l=0}^k \binom{k}{l} B_3^{k-l} \frac{1}{(1-bz)^l} B_4^l \right) \\
&= \sum_{j=0}^n \sum_{k=0}^j \sum_{l=0}^k \binom{n}{j} \binom{j}{k} \binom{k}{l} \frac{1}{(1-bz)^{j+k+l}} B_1^{n-j} B_2^{j-k} B_3^{k-l} B_4^l,
\end{aligned}$$

we have

$$\begin{aligned}
r\left(\frac{t}{n}z\right)^n &= \sum_{j=0}^n \sum_{k=0}^j \sum_{l=0}^k \binom{n}{j} \binom{j}{k} \binom{k}{l} B_1^{n-j} B_2^{j-k} B_3^{k-l} B_4^l \frac{1}{(1-\frac{bt}{n}z)^{j+k+l}} \\
&= \sum_{j=0}^n \sum_{k=0}^j \sum_{l=0}^k \binom{n}{j} \binom{j}{k} \binom{k}{l} B_1^{n-j} B_2^{j-k} B_3^{k-l} B_4^l \left(\frac{n}{bt}\right)^{j+k+l} \frac{1}{(\frac{n}{bt} - z)^{j+k+l}}.
\end{aligned}$$

It follows from Theorem 2.1 that $E(n, t, u) :=$

$$\left\| B_1^n u_0 + \sum_{j=1}^n \sum_{k=0}^j \sum_{l=0}^k \binom{n}{j} \binom{j}{k} \binom{k}{l} B_1^{n-j} B_2^{j-k} B_3^{k-l} B_4^l \left(\frac{n}{bt}\right)^{j+k+l} \frac{(-1)^{j+k+l-1}}{(j+k+l-1)!} \hat{u}^{(j+k+l-1)}\left(\frac{n}{bt}\right) - u(t) \right\|_X$$

satisfies

$$E(n, t, u) \leq \begin{cases} C t^k \frac{1}{n^{4k/5}} \|u^{(k)}\|_\infty & \text{if } u, u^{(k)} \in \mathcal{C}_b(\mathbb{R}^+, X) \text{ and } 1 \leq k \leq 5, \\ C \frac{t^4}{n^4} \|u^{(4)}\|_\infty & \text{if } u, u^{(4)} \in C_b(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X) \end{cases}$$

for all $t \geq 0$.

m=6, Restricted Padé - Type{5}. The rational approximation $r_{\{5\}}$

$$\begin{aligned}
r(z) &= \frac{(-b^5 + 5b^4 - 5b^3 + 5b^2 - 5b + 1)z^5 + (5b^4 - 10b^3 + 5b^2 - 5b + 1)z^4}{(1-bz)^5} \\
&= + \frac{(-10b^3 + 10b^2 - 5b + 1)z^3 + (10b^2 - 5b + 1)z^2 - (5b + 1)z + 1}{(1-bz)^5} \\
&= B_1 + \frac{B_2}{1-bz} + \frac{B_3}{(1-bz)^2} + \frac{B_4}{(1-bz)^3} + \frac{B_5}{(1-bz)^4} + \frac{B_6}{(1-bz)^5}
\end{aligned}$$

with $b \approx 0.47326839$, $B_1 = \frac{120b^5 - 600b^4 + 600b^3 - 200b^2 + 25b - 1}{120b^5}$, $B_2 = \frac{360b^4 - 480b^3 + 180b^2 - 24b + 1}{24b^5}$, $B_3 = \frac{-240b^4 + 390b^3 - 162b^2 + 23b - 1}{12b^5}$, $B_4 = \frac{180b^4 - 324b^3 + 146b^2 + 22b + 1}{12b^5}$, $B_5 = \frac{-144b^4 + 276b^3 - 132b^2 + 21b - 1}{24b^5}$, $B_6 = \frac{120b^4 - 240b^3 + 120b^2 - 20b + 1}{120b^5}$ is an \mathcal{A} -stable restricted Padé approximation of e^z of order $m = 6$. Since

$$\begin{aligned}
r(z)^n &= \left(B_1 + \frac{B_2}{1-bz} + \frac{B_3}{(1-bz)^2} + \frac{B_4}{(1-bz)^3} + \frac{B_5}{(1-bz)^4} + \frac{B_6}{(1-bz)^5} \right)^n \\
&= \sum_{j=0}^n \binom{n}{j} B_1^{n-j} \left(\frac{B_2}{1-bz} + \frac{B_3}{(1-bz)^2} + \frac{B_4}{(1-bz)^3} + \frac{B_5}{(1-bz)^4} + \frac{B_6}{(1-bz)^5} \right)^j \\
&= \sum_{j=0}^n \binom{n}{j} B_1^{n-j} \frac{1}{(1-bz)^j} \left(B_2 + \frac{B_3}{1-bz} + \frac{B_4}{(1-bz)^2} + \frac{B_5}{(1-bz)^3} + \frac{B_6}{(1-bz)^4} \right)^j \\
&= \sum_{j=0}^n \binom{n}{j} B_1^{n-j} \frac{1}{(1-bz)^j} \left(\sum_{k=0}^j \binom{j}{k} B_2^{j-k} \left(\frac{B_3}{1-bz} + \frac{B_4}{(1-bz)^2} + \frac{B_5}{(1-bz)^3} + \frac{B_6}{(1-bz)^4} \right)^k \right) \\
&= \sum_{j=0}^n \sum_{k=0}^j \binom{n}{j} \binom{j}{k} B_1^{n-j} B_2^{j-k} \frac{1}{(1-bz)^{j+k}} \left(\sum_{l=0}^k \binom{k}{l} B_3^{k-l} \left(\frac{B_4}{(1-bz)} + \frac{B_5}{(1-bz)^2} + \frac{B_6}{(1-bz)^3} \right)^l \right) \\
&= \sum_{j=0}^n \sum_{k=0}^j \sum_{l=0}^k \binom{n}{j} \binom{j}{k} \binom{k}{l} \frac{1}{(1-bz)^{j+k+l}} B_1^{n-j} B_2^{j-k} B_3^{k-l} \left(\sum_{u=0}^l \binom{l}{u} B_4^{l-u} \left(\frac{B_5}{1-bz} + \frac{B_6}{(1-bz)^2} \right)^u \right) \\
&= \sum_{j=0}^n \sum_{k=0}^j \sum_{l=0}^k \sum_{u=0}^l \binom{n}{j} \binom{j}{k} \binom{k}{l} \binom{l}{u} \frac{1}{(1-bz)^{j+k+l+u}} B_1^{n-j} B_2^{j-k} B_3^{k-l} B_4^{l-u} \left(\sum_{v=0}^u \binom{u}{v} B_5^{u-v} \left(\frac{B_6}{1-bz} \right)^v \right) \\
&= \sum_{j=0}^n \sum_{k=0}^j \sum_{l=0}^k \sum_{u=0}^l \sum_{v=0}^u \binom{n}{j} \binom{j}{k} \binom{k}{l} \binom{l}{u} \binom{u}{v} \frac{1}{(1-bz)^{j+k+l+u+v}} B_1^{n-j} B_2^{j-k} B_3^{k-l} B_4^{l-u} B_5^{u-v} B_6^v
\end{aligned}$$

We have;

$$\begin{aligned}
r\left(\frac{t}{n}z\right)^n &= \sum_{j=0}^n \sum_{k=0}^j \sum_{l=0}^k \sum_{u=0}^l \sum_{v=0}^u \binom{n}{j} \binom{j}{k} \binom{k}{l} \binom{l}{u} \binom{u}{v} \frac{1}{\left(1 - \frac{bt}{n}z\right)^{j+k+l+u+v}} B_1^{n-j} B_2^{j-k} B_3^{k-l} B_4^{l-u} B_5^{u-v} B_6^v \\
&= \sum_{j=0}^n \sum_{k=0}^j \sum_{l=0}^k \sum_{u=0}^l \sum_{v=0}^u \binom{n}{j} \binom{j}{k} \binom{k}{l} \binom{l}{u} \binom{u}{v} \left(\frac{n}{bt}\right)^{j+k+l+u+v} \frac{1}{\left(\frac{n}{bt} - z\right)^{j+k+l+u+v}} B_1^{n-j} B_2^{j-k} B_3^{k-l} B_4^{l-u} B_5^{u-v} B_6^v
\end{aligned}$$

Let $\binom{n}{j} \binom{j}{k} \binom{k}{l} \binom{l}{u} \binom{u}{v} B_1^{n-j} B_2^{j-k} B_3^{k-l} B_4^{l-u} B_5^{u-v} B_6^v := C_{\{j,n,k,l,u,v\}}$, then, it follows from Theorem 2.1 that $E(n, t, u) :=$

$$\left\| B_1^n f_0 + \sum_{j=1}^n \sum_{k=0}^j \sum_{l=0}^k \sum_{u=0}^l \sum_{v=0}^u C_{\{j,n,k,l,u,v\}} \left(\frac{n}{bt}\right)^{j+k+l+u+v} \frac{(-1)^{j+k+l+u+v-1}}{(j+k+l+u+v-1)!} \hat{f}^{(j+k+l+u+v-1)}\left(\frac{n}{bt}\right) - f(t) \right\|$$

satisfies

$$E(n, t, u) \leq \begin{cases} Ct^k \frac{1}{n^{6k/7}} \|u^{(k)}\|_\infty & \text{if } u, u^{(k)} \in \mathcal{C}_b(\mathbb{R}^+, X) \text{ and } 1 \leq k \leq 7, \\ C \frac{t^6}{n^6} \|u^{(6)}\|_\infty & \text{if } u, u^{(6)} \in C_b(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X) \end{cases}$$

for all $t \geq 0$.

2.4 Applications to the Inhomogeneous Abstract Cauchy Problem

In this section we shall illustrate aptitude and efficiency of the rational inversion methods for the study of time-discretization procedures for inhomogeneous abstract Cauchy problems. After collecting the facts and results on the problem and its solutions (classical and mild), we shall compare 'a semigroup approach' to the approximation of solutions of abstract Cauchy problem with approximation results for the solutions of inhomogeneous abstract Cauchy problem obtained via rational inversion methods for the Laplace transform introduced in Section 2.1. In particular, we shall present results on boundedness, uniform continuity and analyticity of the convolution integral which will allow us to apply the inversion procedures on appropriate spaces.

In this section we are interested in solutions of the initial value problem

$$(IACP) \begin{cases} \dot{u}(t) = Au(t) + f(t) & \text{for } t \geq 0, \\ u(0) = x, \end{cases}$$

where $(A, D(A))$ is an operator on Banach space X , $x \in X$ is the initial value, and $f \in L^1_{loc}(\mathbb{R}^+, X)$.

Our assumption is that the homogeneous problem (i.e., $f \equiv 0$), is well-posed so that $(A, D(A))$ generates a strongly continuous semigroup $\{T(t)\}_{t \geq 0}$. In this case, the solution of (IACP) always exists and is given by the *variations of constants formula (or Lagrange formula)*

$$u(t) := T(t)x + \int_0^t T(t-s)f(s) ds. \quad (2.14)$$

If $(A, D(A))$ is the generator of strongly continuous semigroup $\{T(t)\}_{t \geq 0}$ on Banach space X , $x \in X$, and $f \in L^1(\mathbb{R}^+, X)$, then (2.14) is called the *mild* solution of (IACP).

If $u : \mathbb{R}^+ \rightarrow X$ is continuously differentiable with $u(t) \in D(A)$, and (IACP) is valid, then it is called *classical* solution. Evidently, every classical solution is a mild solution and this necessarily implies that (IACP) has at most one solution. To see this, if u is a classical solution then we have

$$u(t) := T(t)x + \int_0^t T(t-s)f(s) ds.$$

Let $g(s) := T(t-s)u(s)$ then,

$$\begin{aligned} \frac{dg}{ds}(s) &= -AT(t-s)u(s) + T(t-s)\dot{u}(s) \\ &= -AT(t-s)u(s) + T(t-s)(Au(s) + f(s)) = T(t-s)f(s) \\ g(t) - g(0) &= u(t) - T(t)x = \int_0^t T(t-s)f(s)ds. \end{aligned}$$

On the other hand, every mild solution is not necessarily a classical solution. We need to impose further conditions on f so that, for $x \in D(A)$, the mild solution becomes a classical solution. To see this, let A be the generator of a strongly continuous semigroup $\{T(t)\}_{t \geq 0}$ and $x \in X$ such that $T(t)x \notin D(A)$ for any $t \geq 0$. If we define $f(s) := T(s)x$ then, $f(s)$ is continuous for $s \geq 0$. Now consider the initial value problem

$$\begin{aligned} \dot{u}(t) &= Au(t) + T(t)x \\ u(0) &= 0. \end{aligned}$$

Even though $u(0) = 0 \in D(A)$, the proposed mild solution

$$u(t) = \int_0^t T(t-s)T(s)x ds = tT(t)x$$

can not be the classical solution since $tT(t)x$ is not differentiable for $t > 0$. There are many regularity conditions derived for (IACP) to ensure that mild solutions are classical. Here, we just

give the following well-known result; the proof of the statement and the other 'possible' conditions that can be imposed on the function f (or on the semigroup $T(\cdot)$) can be found in, for example, [2], [41], or [46].

Proposition 2.5. *Let $(A, D(A))$ be the generator of a strongly continuous semigroup $\{T(t)\}_{t \geq 0}$ on a Banach space X . If $f(\cdot)$ is continuously differentiable on \mathbb{R}^+ , then (IACP) has a classical solution $u(\cdot)$ on \mathbb{R}^+ for every $x \in D(A)$.*

A key ingredient in the study of the inhomogeneous Cauchy problem is the investigation of the regularity and growth properties of the convolution operator

$$(T * f) : t \mapsto \int_0^t T(t-s)f(s) ds.$$

More precisely, in order to be able to apply the results of the previous section, we are seeking conditions on the semigroup $\{T(t)\}_{t \geq 0}$ and the forcing term $f(\cdot)$ which ensure that the convolution $T * f$ is in $C_b(\mathbb{R}^+, X)$. This can be achieved by 'non-resonance' conditions and some additional assumptions. Let $\{T(t)\}_{t \geq 0}$ be a bounded strongly continuous semigroup on a Banach space X with generator A and we define the *half-line spectrum* of a Laplace transformable function $f \in L^1_{loc}(\mathbb{R}^+, X)$ by

$$sp(f) := \{\eta \in \mathbb{R} : \hat{f} \text{ does not have a analytic extension to an open neighborhood of } i\eta \text{ in } \mathbb{C}\}$$

and the *exponential growth bound* of $T(\cdot)$ by

$$\omega(T) := \inf\{\omega \in \mathbb{R} : \exists M_\omega \text{ such that } \|T(t)\| \leq M_\omega e^{\omega t} \text{ for all } t \geq 0\}.$$

Assuming that $\omega(T) < 0$, one can conclude easily that for $f \in L^\infty(\mathbb{R}^+, X)$, the convolution $T * f$ is bounded, and for $f \in C_{ub}(\mathbb{R}^+, X)$, $T * f \in C_{ub}(\mathbb{R}^+, X)$ (for a proof, see [2]). On

the other hand, assuming $\{T(t)\}_{t \geq 0}$ is bounded, then it was shown by Datko [13] that there exist bounded f such that $T * f$ is unbounded. For example, if $f(t) = T(t) = e^{i\eta t}x$ for all $t \geq 0$, then $(T * f)(t) = te^{i\eta t}x$ and this is unbounded if $x \neq 0$ since there is resonance between $T(\cdot)$ and $f(\cdot)$, reflected in the fact that $i\eta \in \sigma(A) \cap \text{isp}(f)$. Therefore, in order to obtain boundedness of the convolution $T * f$ we need to put some constraints either on the function f or we may require some non-resonance condition by assuming that $\sigma(A) \cap \text{isp}(f) = \emptyset$. Indeed, Datko [13] showed that the mere non-resonance condition is not sufficient.

Let $\{T(t)\}_{t \geq 0}$ be a bounded strongly continuous semigroup on a Banach space X with generator A . $\{T(t)\}_{t \geq 0}$ is said to be uniformly exponentially stable if $\omega(T) < 0$.

The operator $(A, D(A))$ is said to have an L^p -resolvent for some $1 \leq p < \infty$ if there exists $\alpha \in \mathbb{R}$ and $b \geq 0$ such that $\{\alpha + i\eta : |\eta| \geq b\} \subseteq \rho(A)$ and

$$\int_{|\eta| \geq b} \|R(\alpha + i\eta, A)\|^p < \infty.$$

For a proof of the following theorem, see [2], [5], [6].

Theorem 2.6. *Let $\{T(t)\}_{t \geq 0}$ be a bounded, strongly continuous semigroup on a Banach space X with generator $(A, D(A))$.*

- (i) *If $f \in L^1(\mathbb{R}^+, X)$, then $(T * f) \in C_{ub}(\mathbb{R}^+, X)$.*
- (ii) *If $f \in L^\infty(\mathbb{R}^+, X)$ and $T(t)$ is uniformly exponentially stable then $(T * f) \in C_b(\mathbb{R}^+, X)$.*
- (iii) *Let $f \in L^\infty(\mathbb{R}^+, X)$ and suppose that $\sigma(A) \cap \text{isp}(f)$ is empty. If A has an L^p -resolvent for some $1 \leq p < \infty$, then $(T * f) \in C_{ub}(\mathbb{R}^+, X)$.*

Now, we present a semigroup approach in order to find mild and classical solutions of (IACP). The methodology is first to find a proper state space \mathcal{X} and a new operator $(\mathfrak{A}, D(\mathfrak{A}))$ that generates a new semigroup $\{\mathfrak{T}(t)\}_{t \geq 0}$ on \mathcal{X} .

Let $(A, D(A))$ be the generator of strongly continuous semigroup $\{T(t)\}_{t \geq 0}$, $\mathcal{X} := X \times C_0(\mathbb{R}^+, X)$, and let us define

$$\mathfrak{T}(t) := \begin{pmatrix} T(t) & R(t) \\ 0 & S(t) \end{pmatrix},$$

where $\{S(t)\}_{t \geq 0}$ is the (left) shift semigroup on $C_0(\mathbb{R}^+, X)$, $S(t)f(x) = f(x + t)$ and $R(t) : C_0(\mathbb{R}^+, X) \rightarrow X$ is defined as

$$R(t)f := \int_0^t T(t-s)f(s) ds \quad \text{for } f \in C_0(\mathbb{R}^+, X).$$

It is easy to see that $\{\mathfrak{T}(t)\}_{t \geq 0}$ is a strongly continuous semigroup on \mathcal{X} . Indeed, the semigroup property $\mathfrak{T}(t+s) = \mathfrak{T}(t)\mathfrak{T}(s)$ follows from

$$\begin{aligned} T(t)R(s)f + R(t)S(s) &= T(t) \int_0^s T(s-r)f(r) dr + \int_0^t T(t-r)S(s)f(r) dr \\ &= \int_0^s T(t+s-r)f(r) dr + \int_s^{t+s} T(t+s-r)f(r) dr \\ &= R(t+s)f \quad \text{for all } t, s > 0. \end{aligned}$$

The strong continuity of $\{\mathfrak{T}(t)\}_{t \geq 0}$ follows since $\lim_{t \rightarrow 0} R(t)f = 0$ for every $f \in C_0(\mathbb{R}^+, X)$.

The generator $(\mathfrak{A}, D(\mathfrak{A}))$ of $\{\mathfrak{T}(t)\}_{t \geq 0}$ is given by

$$\mathfrak{A} \begin{pmatrix} x \\ f \end{pmatrix} := \begin{pmatrix} Ax + f(0) \\ f' \end{pmatrix}$$

for $\begin{pmatrix} x \\ f \end{pmatrix} \in D(\mathfrak{A}) := D(A) \times C_0^1(\mathbb{R}^+, X)$, or in matrix notation

$$\mathfrak{A} = \begin{pmatrix} A & \delta_0 \\ 0 & d/ds \end{pmatrix},$$

where δ_0 is the point evaluation in 0. To see this, we first compute the resolvent

$$R(\lambda, \mathfrak{A}) := \int_0^\infty e^{-\lambda r} \mathfrak{T}(r) dr = \begin{pmatrix} R(\lambda, A) & Q(\lambda) \\ 0 & R(\lambda, d/ds) \end{pmatrix},$$

where

$$Q(\lambda)f := \int_0^\infty e^{-\lambda t} R(t)f dt = R(\lambda, A) \int_0^\infty e^{-\lambda r} f(r) dr \quad \text{for } f \in C_0(\mathbb{R}^+, X).$$

On the other hand, by a straightforward computation

$$\left[\lambda - \begin{pmatrix} A & \delta_0 \\ 0 & d/ds \end{pmatrix} \right]^{-1} = \begin{pmatrix} R(\lambda, A) & R(\lambda, A)\delta_0 R(\lambda, d/ds) \\ 0 & R(\lambda, d/ds) \end{pmatrix}. \quad (2.15)$$

Now, since the resolvent of the shift semigroup $R(\lambda, d/ds)f(s) = \int_0^\infty e^{-\lambda(t-s)} f(t) dt$, we have

$$Q(\lambda) = R(\lambda, A)\delta_0 R(\lambda, d/ds).$$

That is, the resolvents coincide and

$$\mathfrak{A} \begin{pmatrix} x \\ f \end{pmatrix} := \begin{pmatrix} Ax + f(0) \\ f' \end{pmatrix}$$

is the generator of the strongly continuous semigroup $\{\mathfrak{T}(t)\}_{t \geq 0}$.

In order to obtain mild and classical solutions, for $\begin{pmatrix} x \\ f \end{pmatrix} \in \mathcal{X}$, let

$$\mathbf{u}(t) = \begin{pmatrix} u_1(t) \\ u_2(t) \end{pmatrix} := \mathfrak{T}(t) \begin{pmatrix} x \\ f \end{pmatrix} = \begin{pmatrix} T(t)x + R(t)f \\ S(t)f \end{pmatrix}.$$

Then $\mathbf{u}(\cdot)$ is the mild solution of the abstract Cauchy problem

$$\begin{aligned} \mathbf{u}'(t) &= \mathfrak{A}\mathbf{u}(t) \quad \text{for } t > 0, \\ \mathbf{u}(0) &= \begin{pmatrix} x \\ f \end{pmatrix}. \end{aligned}$$

In the case, $\begin{pmatrix} x \\ f \end{pmatrix} \in D(\mathfrak{A})$,

$$u_1'(t) = Au_1(t) + \delta_0 u_2(t) = Au_1(t) + f(t),$$

and therefore,

$$u_1(t) = T(t)x + R(t)f = T(t)x + \int_0^t T(t-s)f(s) ds$$

is the classical solution of (IACP).

Now we are ready to obtain error estimates for the approximation of solutions of (IACP) by using the rational approximation schemes for operator semigroups (for details see Section 1.3). More precisely, in the following we make use of the \mathcal{A} -stable backward Euler scheme and the Brenner-Thomée result (Theorem 1.8) for the strongly continuous semigroup $\{\mathfrak{T}(t)\}_{t \geq 0}$ generated by the operator $(\mathfrak{A}, D(\mathfrak{A}))$ on the new state space \mathcal{X} . We have

$$V_{BE} \left(\frac{t}{n} \right)^n \begin{pmatrix} x \\ f \end{pmatrix} = \left(I - \frac{t}{n} \mathfrak{A} \right)^{-n} \begin{pmatrix} x \\ f \end{pmatrix} = \left(\frac{n}{t} R\left(\frac{n}{t}, \mathfrak{A}\right) \right)^n \begin{pmatrix} x \\ f \end{pmatrix} \longrightarrow \mathfrak{T}(t) \begin{pmatrix} x \\ f \end{pmatrix}.$$

An easy induction shows that

$$R(\lambda, \mathfrak{A})^n = \begin{pmatrix} R(\lambda, A)^n & R(\lambda, A) \left[\sum_{j=0}^{n-1} R(\lambda, A)^{n-j} \delta_0 R(\lambda, d/ds)^j \right] R(\lambda, d/ds) \\ 0 & R(\lambda, d/ds)^n \end{pmatrix}.$$

Since the resolvent $R(\lambda, d/ds)$ is the Laplace transform of the shift semigroup $\{S(t)\}_{t \geq 0}$,

$$R(\lambda, d/ds)f(x) = \int_0^\infty e^{-\lambda t} f(x+t) dt,$$

and δ_0 is the point evaluation in 0, we have

$$\delta_0 R(\lambda, d/ds)f = \int_0^\infty e^{-\lambda t} f(t) dt = \hat{f}(\lambda).$$

Since all resolvents satisfy the formula

$$R(\lambda, d/ds)^{n+1} = (-1)^n \frac{1}{n!} R(\lambda, d/ds)^{(n)},$$

it follows that

$$\begin{aligned} R(\lambda, d/ds)^{n+1} f(x) &= (-1)^n \frac{1}{n!} \frac{d^n}{d\lambda^n} \int_0^\infty e^{-\lambda t} T(t) f(x) dt \\ &= \int_0^\infty e^{-\lambda t} \frac{t^n}{n!} f(x+t) dt. \end{aligned}$$

Thus

$$\begin{aligned} \delta_0 R(\lambda, d/ds)^{n+1} f &= \int_0^\infty e^{-\lambda t} \frac{t^n}{n!} f(t) dt \\ &= \frac{(-1)^n}{n!} \hat{f}^{(n)}(\lambda) =: a_{n+1}(\lambda). \end{aligned}$$

Now, if we assume that $\|\mathfrak{T}(t)\| \leq M$ (which is the case, for example, if $w(T) < 0$), then we can use the Brenner-Thomée result (Theorem 1.8) for $\omega = 0$ and get

$$\begin{aligned} &\left\| \left(\frac{n}{t}\right)^n \sum_{j=0}^n R\left(\frac{n}{t}, A\right)^{n+1-j} a_{j+1}\left(\frac{n}{t}\right) - \int_0^t T(t-s) f(s) ds \right\| \\ &= \left\| \left[\sum_{j=0}^n \left(\frac{n}{t}\right)^{n+1-j} R\left(\frac{n}{t}, A\right)^{n+1-j} \right] \left[\left(\frac{n}{t}\right)^{j+1} a_{j+1}\left(\frac{n}{t}\right) \right] - \int_0^t T(t-s) f(s) ds \right\|. \end{aligned}$$

That is,

$$\left\| \left(\frac{n}{t}\right)^n R\left(\frac{n}{t}, \mathfrak{A}\right)^n \begin{pmatrix} x \\ f \end{pmatrix} - \mathfrak{T}(t) \begin{pmatrix} x \\ f \end{pmatrix} \right\| \leq C t^2 \frac{1}{n} \|\mathfrak{A}^2 \begin{pmatrix} x \\ f \end{pmatrix}\|,$$

where

$$\mathfrak{A}^2 \begin{pmatrix} x \\ f \end{pmatrix} = \begin{pmatrix} A^2 x + A\delta_0 f + \delta_0 d/ds f \\ \frac{d^2 f}{ds^2} \end{pmatrix}.$$

Thus,

$$\left\| \left(\frac{n}{t}\right)^n \sum_{j=0}^n R\left(\frac{n}{t}, A\right)^{n+1-j} a_{j+1}\left(\frac{n}{t}\right) - \int_0^t T(t-s)f(s) ds \right\| \leq (\|Af(0) + f'(0)\| + \|f''\|) \frac{c}{n} t^2.$$

In the remainder of this section we explore mild solutions of the inhomogeneous abstract Cauchy problem in two different settings; on the half-line \mathbb{R}^+ and on the sector Σ_θ . In order to be able to apply rational inversion methods, (see Theorem 2.1) to approximate solutions of the inhomogeneous Cauchy problem, we shall need to investigate boundedness, uniform continuity and the analyticity of the convolution integral on these domains.

Let A generate a bounded strongly continuous semigroup $\{T(t)\}_{t \geq 0}$ on a Banach space X and let $f \in L^1_{loc}(\mathbb{R}^+, X)$, then the mild solution of the inhomogeneous abstract Cauchy problem

$$(IACP) \begin{cases} \dot{u}(t) = Au(t) + f(t) & \text{for } t \geq 0, \\ u(0) = 0 \end{cases}$$

is given, as we already pointed out in (2.14), by the variations of constants formula

$$u(t) = (T * f)(t) = \int_0^t T(t-s)f(s) ds \quad (2.16)$$

If we apply the Laplace transform to (IACP), we get

$$\begin{aligned} \lambda \hat{u}(\lambda) &= A\hat{u}(\lambda) + \hat{f}(\lambda), \text{ or} \\ \hat{u}(\lambda) &= R(\lambda, A)\hat{f}(\lambda). \end{aligned}$$

This shows that (2.16) in fact, is the inverse Laplace transform of $\hat{u}(\lambda) = R(\lambda, A)\hat{f}(\lambda)$ and can be approximated using any of the rational inversion methods for the Laplace transform presented

earlier. However, it has to be pointed out that in order to use these results one has to know a priori that the unknown solution u is either in $C_0(\mathbb{R}^+, X)$, or $C_b(\mathbb{R}^+, X)$, or $C_{ub}(\mathbb{R}^+, X)$ (and for this one needs non-resonance results like the ones presented in Theorem 2.6).

Clearly, one can easily adopt the Brenner-Thomée results to the shift semigroup on

$$C_b^\omega(\mathbb{R}^+, X) := \{f : [0, \infty) \rightarrow X : r \mapsto e^{-\omega r} f(r) \in C_b([0, \infty), X)\}$$

with

$$\|f\|_\omega := \sup_{r \geq 0} \|e^{-\omega r} f(r)\|.$$

Then the shift semigroup satisfies

$$\begin{aligned} \|T(t)f\|_\omega &= \sup_{r \geq 0} \|e^{-\omega r} T(t)f(r)\| = \sup_{r \geq 0} \|e^{-\omega r} f(t+r)\| \\ &= \sup_{r \geq 0} \|e^{\omega t} e^{-\omega(r+t)} f(t+r)\| \\ &= e^{\omega t} \sup_{r \geq 0} \|e^{-\omega(r+t)} f(t+r)\| \\ &= e^{\omega t} \sup_{r \geq t} \|e^{-\omega r} f(r)\| \leq e^{\omega t} \sup_{r \geq 0} \|e^{-\omega r} f(r)\| \\ &= e^{\omega t} \|f\|_\omega \end{aligned}$$

and we can apply the Brenner-Thomée Theorem 1.8 to our inversion formulas for the Laplace transform by picking up the term $e^{c\omega t}$ from equation (1.27) in our error estimates. However, it goes without further explanation, that an additional error term of the form $e^{c\omega t}$ should be avoided if at all possible.

Now, we will look at the convolution $T * f$ on a sector $\Sigma_\theta := \{z \in \mathbb{C} - \{0\} : |\arg(z)| < \theta\}$ in the complex plane of angle $\theta \in (0, \pi]$ where $\{T(z)\}_{z \in \Sigma_\theta \cup \{0\}}$ is a bounded analytic semigroup and

$f : \Sigma_\theta \rightarrow X$ is an analytic function. In order to apply rational inversion procedures (Theorem 2.1) we need to have that $(T * f) \in C_b(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X)$.

First, we state an important variant of the well-known 'maximum-modulus theorem' which was given by Phragmén and Lindelöf. For a proof, see for example [54].

Theorem 2.7 (Phragmén-Lindelöf). *Let $\Sigma_{\pi/\theta}$ be a sector where $\theta > 1$. Suppose that $h : \overline{\Sigma_{\pi/\theta}} \rightarrow X$ is continuous on $\overline{\Sigma_{\pi/\theta}}$ and analytic on $\Sigma_{\pi/\theta}$. Suppose also that $h(\cdot)$ is bounded on the boundary of $\Sigma_{\pi/\theta}$; i.e.,*

$$\|h(r e^{\mp i\pi/\theta})\| \leq M \quad \text{for all } r > 0.$$

If for all $\epsilon > 0$, there exists a positive constant K_ϵ such that

$$|h(z)| \leq K_\epsilon e^{\epsilon|z|^{\theta/2}} \quad \text{for every } \epsilon > 0,$$

and for all z with $|z|$ sufficiently large, then $|h(z)| \leq K_\epsilon$ for all $z \in \Sigma_{\pi/\theta}$.

Now assume that $T : \Sigma_\theta \rightarrow L(X)$ is a bounded analytic semigroup (strongly continuous or bi-continuous) and that $f \in C(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X)$. Then

$$\Psi : z \rightarrow \int_0^z T(z-s)f(s) ds := \int_0^1 T(z-tz)f(tz) z dt = \int_0^1 h(t, z) dt,$$

where

$$h(t, z) := T(z-tz)f(tz) z$$

is analytic. To see this, first observe that $z \mapsto h(t, z)$ is analytic on Σ_θ for all $t \in [0, 1]$, and that $t \mapsto h(t, z)$ is continuous on $[0, 1]$ for all $z \in \mathbb{C}$. But then, since

$$\begin{aligned}
\int_{\Gamma} \Psi(z) dz &= \int_{\Gamma} \int_0^1 h(t, z) dt dz \\
&= \int_0^1 \int_{\Gamma} h(t, z) dz dt = 0
\end{aligned}$$

for all closed curves Γ in Σ_{θ} , it follows from Cauchy's theorem that Ψ is analytic.

As the convolution of a bounded analytic operator and an analytic function is again analytic, what remains to show is that the boundedness of the convolution $T * f$ on the sector Σ_{θ} which will then allow us to use rational inversion methods to approximate solutions of the inhomogeneous abstract Cauchy problem.

Let $\{T(z)\}_{z \in \Sigma_{\pi/\theta} \cup \{0\}}$ ($\theta > 1$) be a bounded analytic semigroup with $\|T(z)\| \leq M$, $f : \Sigma_{\pi/\theta} \rightarrow X$ be an analytic function and $t \mapsto f(te^{\mp i\pi/\theta}) \in L^1((0, \infty), X)$. In order to prove boundedness on the boundary of the sector, $\partial\Sigma_{\pi/\theta}$, let $\gamma := \frac{\pi}{\theta}$, $\theta > 1$ and for arbitrary $t > 0$ consider

$$h(te^{i\gamma}) = \int_0^{te^{i\gamma}} T(te^{i\gamma} - s) f(s) ds$$

and let $s := \omega \cdot e^{i\gamma}$, then

$$\begin{aligned}
h(te^{i\gamma}) &= \int_0^t T(te^{i\gamma} - \omega e^{i\gamma}) f(\omega e^{i\gamma}) e^{i\gamma} d\omega \\
&= e^{i\gamma} \int_0^t T(e^{i\gamma}(t - \omega)) f(\omega e^{i\gamma}) d\omega \\
&= e^{i\gamma} \int_0^t T_{\gamma}(t - \omega) f_{\gamma}(\omega) d\omega.
\end{aligned}$$

Since $T_{\gamma}(\cdot)$ is bounded strongly continuous semigroup and $f \in L^1(\Sigma_{\pi/\theta}, X)$, it follows that $h(\cdot)$ is bounded on $\partial\Sigma_{\pi/\theta}$.

Now, in order to make use of Phragmén-Lindelöf theorem, we need necessary conditions on $f(\cdot)$ (or $T(\cdot)$) so that the convolution $h = T * f$ would satisfy

$$\|h(z)\| \leq K_\epsilon e^{\epsilon \cdot |z|^{\theta/2}}.$$

Suppose that for all $\epsilon > 0$, there exists a constant K_ϵ such that

$$\|f(z)\| \leq K_\epsilon e^{\epsilon \cdot |z|^{\theta/2}}$$

holds. Then

$$\begin{aligned} \|h(z)\| &= \left\| \int_0^z T(z-s)f(s) ds \right\| = \left\| \int_0^{|z|} T(|z|e^{i\epsilon} - |s|e^{i\epsilon}) f(se^{i\epsilon}) e^{i\epsilon} ds \right\| \\ &\leq M \cdot |z| K_\epsilon e^{\epsilon \cdot |z|^{\theta/2}} = \tilde{K}_\epsilon e^{\tilde{\epsilon} \cdot |z|^{\theta/2}}. \end{aligned}$$

Therefore, we have that the conditions of (i) of Theorem (2.1) are satisfied and we can apply rational Laplace transform inversion methods to approximate solutions of the inhomogeneous abstract Cauchy problem.

For example, if one considers $r(z) = \frac{1}{1-z}$ (i.e., the Backward Euler or Post-Widder Inversion of the Laplace Transform), then the error

$$\begin{aligned} E(n, u, t) &:= \left\| \frac{(-1)^{n-1}}{(n-1)!} \left(\frac{n}{t}\right)^n \hat{u}^{(n-1)}\left(\frac{n}{t}\right) - u(t) \right\| \\ &= \left\| \frac{(-1)^{n-1}}{(n-1)!} \left(\frac{n}{t}\right)^n \sum_{j=0}^{n-1} \binom{n-1}{j} R\left(\frac{n}{t}, A\right)^{n-1-j} \hat{f}^{(j)}\left(\frac{n}{t}\right) - u(t) \right\| \end{aligned}$$

satisfies $E(n, t, u) \leq Ct \frac{1}{\sqrt{n}} \|u'\|_\infty$ if u is a classical solution of (IACP) and $E(n, t, u) \leq C \frac{1}{n} \|u\|_\infty$ if $u \in C_b(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X)$.

If one takes higher order rational Laplace transform inversions like Padé-{10,11} Inversion of the Laplace Transform mentioned above and if one is assured that $u \in C_b(\overline{\Sigma_\theta}, X) \cap H(\Sigma_\theta, X)$, then the speed of convergence can be increased dramatically while at the same time lower powers

of $R(\frac{n}{t}, A)$ and fewer derivatives of \hat{f} are required. However, if u is ‘just’ a classical solution of (IACP) that possesses no additional regularity beyond being a C^1 -function, then none of the rational Laplace Transform inversion methods provides any advantage over the Post-Widder inversion (2.17). In this case, the stabilization methods of McAllister and Neubrandner [42] allow us to modify higher order rational Laplace Transform inversion methods so that the modified higher order schemes converge like $O(\frac{1}{n})$ for classical solutions of (IACP).

Similarly, if $\{T(z)\}_{z \in \Sigma_{\pi/\theta} \cup \{0\}}$ ($\theta > 1$) is a bounded analytic semigroup with $\|T(z)\| \leq M$, $f : \Sigma_{\pi/\theta} \rightarrow X$ analytic, $|f(z)| \leq K_\epsilon e^{\epsilon \cdot |z|^{\theta/2}}$ for all $\epsilon > 0$ and $z \in \Sigma_{\pi/\theta}$, $\sigma(A) \cap \text{isp}(f) = \emptyset$, and $t \mapsto f(te^{\mp i\pi/\theta}) \in L^\infty((0, \infty), X)$, then one can use again the Phragmén-Lindelöf Theorem 2.7 in combination with the non-resonance Theorem 2.6 to obtain that $u \in C_b(\overline{\Sigma}_{\pi/\theta}, X)$.

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Vita

Koray Özer, was born in September, 1977, in Adana, Turkey. He finished his studies with a Bachelor of Science degree in mathematics at Koç University, Istanbul, Turkey in May 2000. In August 2002, he came to Louisiana State University to pursue graduate studies in mathematics. He received a Master of Science degree in mathematics from Louisiana State University in May 2004. He is currently a candidate for the degree of Doctor of Philosophy in mathematics, which will be awarded in August 2008.